Fundamentals of Optimization Theory
With Applications to Machine Learning

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Chapter 1

Introduction

In recent years, computer vision, robotics, machine learning, and data science have been some of the key areas that have contributed to major advances in technology. Anyone who looks at papers or books in the above areas will be baffled by a strange jargon involving exotic terms such as kernel PCA, ridge regression, lasso regression, support vector machines (SVM), Lagrange multipliers, KKT conditions, etc. Do support vector machines chase cattle to catch them with some kind of super lasso? No! But one will quickly discover that behind the jargon which always comes with a new field (perhaps to keep the outsiders out of the club), lies a lot of “classical” linear algebra and techniques from optimization theory. And there comes the main challenge: in order to understand and use tools from machine learning, computer vision, and so on, one needs to have a firm background in linear algebra and optimization theory. To be honest, some probability theory and statistics should also be included, but we already have enough to contend with.

Many books on machine learning struggle with the above problem. How can one understand what are the dual variables of a ridge regression problem if one doesn’t know about the Lagrangian duality framework? Similarly, how is it possible to discuss the dual formulation of SVM without a firm understanding of the Lagrangian framework?

The easy way out is to sweep these difficulties under the rug. If one is just a consumer of the techniques we mentioned above, the cookbook recipe approach is probably adequate. But this approach doesn’t work for someone who really wants to do serious research and make significant contributions. To do so, we believe that one must have a solid background in linear algebra and optimization theory.

This is a problem because it means investing a great deal of time and energy studying these fields, but we believe that perseverance will be amply rewarded.

This second volume covers some elements of optimization theory and applications, especially to machine learning. This volume is divided in five parts:

(1) Preliminaries of Optimization Theory.

(2) Linear Optimization.
CHAPTER 1. INTRODUCTION

(3) Nonlinear Optimization.

(4) Applications to Machine Learning.


Part I is devoted to some preliminaries of optimization theory. The goal of most optimization problems is to minimize (or maximize) some objective function $J$ subject to equality or inequality constraints. Therefore it is important to understand when a function $J$ has a minimum or a maximum (an optimum). If the function $J$ is sufficiently differentiable, then a necessary condition for a function to have an optimum typically involves the derivative of the function $J$, and if $J$ is real-valued, its gradient $\nabla J$.

Thus it is desirable to review some basic notions of topology and calculus, in particular, to have a firm grasp of the notion of derivative of a function between normed vector spaces. Partial derivatives $\partial f/\partial A$ of functions whose range and domain are spaces of matrices tend to be used casually, even though in most cases a correct definition is never provided. It is possible, and simple, to define rigorously derivatives, gradients, and directional derivatives of functions defined on matrices and to avoid these nonsensical partial derivatives.

Chapter 19 contains a review of basic topological notions used in analysis. We pay particular attention to complete metric spaces and complete normed vector spaces. In fact, we provide a detailed construction of the completion of a metric space (and of a normed vector space) using equivalence classes of Cauchy sequences. Chapter 20 is devoted to some notions of differential calculus, in particular, directional derivatives, total derivatives, gradients, Hessians, and the inverse function theorem.

Chapter 21 deals with extrema of real-valued functions. In most optimization problems, we need to find necessary conditions for a function $J: \Omega \to \mathbb{R}$ to have a local extremum with respect to a subset $U$ of $\Omega$ (where $\Omega$ is open). This can be done in two cases:

(1) The set $U$ is defined by a set of equations,

$$U = \{x \in \Omega \mid \varphi_i(x) = 0, \ 1 \leq i \leq m\},$$

where the functions $\varphi_i: \Omega \to \mathbb{R}$ are continuous (and usually differentiable).

(2) The set $U$ is defined by a set of inequalities,

$$U = \{x \in \Omega \mid \varphi_i(x) \leq 0, \ 1 \leq i \leq m\},$$

where the functions $\varphi_i: \Omega \to \mathbb{R}$ are continuous (and usually differentiable).

In (1), the equations $\varphi_i(x) = 0$ are called equality constraints, and in (2), the inequalities $\varphi_i(x) \leq 0$ are called inequality constraints. The case of equality constraints is much easier to deal with and is treated in Chapter 21.
If the functions \( \varphi_i \) are convex and \( \Omega \) is convex, then \( U \) is convex. This is a very important case that we will discuss later. In particular, if the functions \( \varphi_i \) are affine, then the equality constraints can be written as \( Ax = b \), and the inequality constraints as \( Ax \leq b \), for some \( m \times n \) matrix \( A \) and some vector \( b \in \mathbb{R}^m \). We will also discuss the case of affine constraints later.

In the case of equality constraints, a necessary condition for a local extremum with respect to \( U \) can be given in terms of Lagrange multipliers. In the case of inequality constraints, there is also a necessary condition for a local extremum with respect to \( U \) in terms of generalized Lagrange multipliers and the Karush–Kuhn–Tucker conditions. This will be discussed in Chapter 31.

In Chapter 22 we discuss Newton’s method and some of its generalizations (the Newton–Kantorovich theorem). These are methods to find the zeros of a function.

Chapter 23 covers the special case of determining when a quadratic function has a minimum, subject to affine equality constraints. A complete answer is provided in terms of the notion of symmetric positive semidefinite matrices.

The Schur complement is introduced in Chapter 24. We give a complete proof of a criterion for a matrix to be positive definite (or positive semidefinite) stated in Boyd and Vandenberghe [22] (Appendix B).

Part II deals with the special case where the objective function is a linear form and the constraints are affine inequality and equality constraints. This subject is known as linear programming, and the next four chapters give an introduction to the subject. Although linear programming has been supplanted by convex programming and its variants, it is still a great workhorse. It is also a great warm up for the general treatment of Lagrangian duality. We pay particular attention to versions of Farkas’ lemma, which is at the heart of duality in linear programming.

Part III is devoted to nonlinear optimization, which is the case where the objective function \( J \) is not linear and the constraints are inequality constraints. Since it is practically impossible to say anything interesting if the constraints are not convex, we quickly consider the convex case.

In optimization theory one often deals with function spaces of infinite dimension. Typically, these spaces either are Hilbert spaces or can be completed as Hilbert spaces. Thus it is important to have some minimum knowledge about Hilbert spaces, and we feel that this minimum knowledge includes the projection lemma, the fact that a closed subset has an orthogonal complement, the Riesz representation theorem, and a version of the Farkas–Minkowski lemma. Chapter 29 covers these topics. A more detailed introduction to Hilbert spaces is given in Appendix A.

Chapter 30 is devoted to some general results of optimization theory. A main theme is to find sufficient conditions that ensure that an objective function has a minimum which is achieved. We define the notion of a coercive function. The most general result is Theorem 30.2, which applies to a coercive convex function on a convex subset of a separable
Hilbert space. In the special case of a coercive quadratic functional, we obtain the Lions–
Stampacchia theorem (Theorem 30.5), and the Lax–Milgram theorem (Theorem 30.6). We
define elliptic functionals, which generalize quadratic functions defined by symmetric posi-
tive definite matrices. We define gradient descent methods, and discuss their convergence.
We also present the method of conjugate gradients and prove its correctness. We briefly
discuss the method of gradient projection and the penalty method in the case of constrained
optima.

Chapter 31 contains the most important results of nonlinear optimization theory. We
begin by defining the cone of feasible directions and then state a necessary condition for a
function to have local minimum on a set $U$ that is not necessarily convex in terms of the
cone of feasible directions. The cone of feasible directions is not always convex, but it is if
the constraints are inequality constraints. An inequality constraint $\varphi(u) \leq 0$ is said to be
active if $\varphi(u) = 0$. One can also define the notion of qualified constraint. Theorem 31.5
gives necessary conditions for a function $J$ to have a minimum on a subset $U$ defined by
qualified inequality constraints in terms of the Karush–Kuhn–Tucker conditions (for short
KKT conditions), which involve nonnegative Lagrange multipliers. The proof relies on a
version of the Farkas–Minkowski lemma. Some of the KTT conditions assert that $\lambda_i \varphi_i(u) = 0$, where $\lambda_i \geq 0$ is the Lagrange multiplier associated with the constraint $\varphi_i \leq 0$. To some
extent, this implies that active constraints are more important than inactive constraints,
since if $\varphi_i(u) < 0$ is an inactive constraint, then $\lambda_i = 0$. In general, the KKT conditions
are useless unless the constraints are convex. In this case, there is a manageable notion of
qualified constraint given by Slater’s conditions. Theorem 31.6 gives necessary conditions
for a function $J$ to have a minimum on a subset $U$ defined by convex inequality constraints
in terms of the Karush–Kuhn–Tucker conditions. Furthermore, if $J$ is also convex and if the
KKT conditions hold, then $J$ has a global minimum.

We illustrate the KKT conditions on an interesting example, the so-called hard margin
support vector machine; see Sections 31.3 and 31.4. The problem is a classification problem,
or more accurately a separation problem. Suppose we have two nonempty disjoint finite sets
of $p$ blue points $\{u_i\}_{i=1}^p$ and $q$ red points $\{v_j\}_{j=1}^q$ in $\mathbb{R}^n$. Our goal is to find a hyperplane $H$
of equation $w^\top x - b = 0$ (where $w \in \mathbb{R}^n$ is a nonzero vector and $b \in \mathbb{R}$), such that all the
blue points $u_i$ are in one of the two open half-spaces determined by $H$, and all the red points
$v_j$ are in the other open half-space determined by $H$.

If the two sets are indeed separable, then in general there are infinitely many hyperplanes
separating them. Vapnik had the idea to find a hyperplane that maximizes the smallest
distance between the points and the hyperplane. Such a hyperplane is indeed unique and
is called a maximal hard margin hyperplane, or hard margin support vector machine. The
support vectors are those for which the constraints are active.

Section 31.5 contains the most important results of the chapter. The notion of Lagrangian
duality is presented. Given a primal optimization problem $(P)$ consisting in minimizing an
objective function $J(v)$ with respect to some inequality constraints $\varphi_i(v) \leq 0$, $i = 1, \ldots, m$,
we define the dual function $G(\mu)$ as the result of minimizing the Lagrangian

$$
L(v, \mu) = J(v) + \sum_{i=1}^{m} \mu_i \varphi_i(v)
$$

with respect to $v$, with $\mu \in \mathbb{R}^m_+$. The dual program (D) is then to maximize $G(\mu)$ with respect to $\mu \in \mathbb{R}^m_+$. It turns out that $G$ is a concave function, and the dual program is an unconstrained maximization. This is actually a misleading statement because $G$ is generally a partial function, so maximizing $G(\mu)$ is equivalent to a constrained maximization problem in which the constraints specify the domain of $G$, but in many cases, we obtain a dual program simpler than the primal program. If $d^*$ is the optimal value of the dual program and if $p^*$ is the optimal value of the primal program, we always have

$$
d^* \leq p^*,
$$

which is known as weak duality. Under certain conditions, $d^* = p^*$, that is, the duality gap is zero, in which case we say that strong duality holds. Also, under certain conditions, a solution of the dual yields a solution of the primal, and if the primal has an optimal solution, then the dual has an optimal solution, but beware that the converse is generally false (see Theorem 31.14). We also show how to deal with equality constraints, and discuss the use of conjugate functions to find the dual function. Our coverage of Lagrangian duality is quite thorough, but we do not discuss more general orderings such as the semidefinite ordering. For these topics which belong to convex optimization, the reader is referred to Boyd and Vandenberghe [22].

The next three chapters constitute Part IV, which covers some applications of optimization theory (in particular Lagrangian duality) to machine learning.

In Chapter 32, we discuss linear regression. This problem can be cast as a learning problem. We observe a sequence of pairs $((x_1, y_1), \ldots, (x_m, y_m))$ called a set of training data, where $x_i \in \mathbb{R}^n$ and $y_i \in \mathbb{R}$, viewed as input-output pairs of some unknown function $f$ that we are trying to infer. The simplest kind of function is a linear function $f(x) = x^\top w$, where $w \in \mathbb{R}^n$ is a vector of coefficients usually called a weight vector. Since the problem is overdetermined and since our observations may be subject to errors, we can’t solve for $w$ exactly as the solution of the system $Xw = y$, so instead we solve the least-squares problem of minimizing $\|Xw - y\|_2^2$. In general, there are still infinitely many solutions so we add a regularizing term. If we add the term $K \|w\|_2^2$ to the objective function $J(w) = \|Xw - y\|_2^2$, then we have ridge regression. This problem is discussed in Section 32.1.

We derive the dual program. The dual has a unique solution which yields a solution of the primal. However, the solution of the dual is given in terms of the matrix $XX^\top$ (whereas the solution of the primal is given in terms of $X^\top X$), and since our data points $x_i$ are represented by the rows of the matrix $X$, we see that this solution only involves inner products of the $x_i$. This observation is the core of the idea of kernel functions, which we introduce. We also explain how to solve the problem of learning an affine function $f(x) = x^\top w + b$. For these topics which belong to convex optimization, the reader is referred to Boyd and Vandenberghe [22].
In general, the vectors $w$ produced by ridge regression have few zero entries. In practice, it is highly desirable to obtain sparse solutions, that is, vectors $w$ with many components equal to zero. This can be achieved by replacing the regularizing term $K\|w\|_2^2$ by the regularizing term $K\|w\|_1$; see Section 32.2. This method has the exotic name of lasso regression. This time, there is no closed-form solution, but this is a convex optimization problem and there are efficient iterative methods to solve it, although we do not discuss such methods here.

Chapter 33 is an introduction to positive definite kernels and the use of kernel functions in machine learning.

Let $X$ be a nonempty set. If the set $X$ represents a set of highly nonlinear data, it may be advantageous to map $X$ into a space $F$ of much higher dimension called the feature space, using a function $\varphi: X \rightarrow F$ called a feature map. This idea is that $\varphi$ “unwinds” the description of the objects in $F$ in an attempt to make it linear. The space $F$ is usually a vector space equipped with an inner product $\langle -, - \rangle$. If $F$ is infinite dimensional, then we assume that it is a Hilbert space.

Many algorithms that analyze or classify data make use of the inner products $\langle \varphi(x), \varphi(y) \rangle$, where $x, y \in X$. These algorithms make use of the function $\kappa: X \times X \rightarrow \mathbb{C}$ given by

$$\kappa(x, y) = \langle \varphi(x), \varphi(y) \rangle, \quad x, y \in X,$$

called a kernel function.

The kernel trick is to pretend that we have a feature embedding $\varphi: X \rightarrow F$ (actually unknown), but to only use inner products $\langle \varphi(x), \varphi(y) \rangle$ that can be evaluated using the original data through the known kernel function $\kappa$. It turns out that the functions of the form $\kappa$ as above can be defined in terms of a condition which is reminiscent of positive semidefinite matrices (see Definition 33.2). Furthermore, every function satisfying Definition 33.2 arises from a suitable feature map into a Hilbert space; see Theorem 33.8.

We illustrate the kernel methods on two examples: (1) kernel PCA (see Section 33.3), and (2) $\nu$-SV Regression, which is a variant of linear regression in which certain points are allowed to be “misclassified” (see Section 33.4).

In Chapter 34 we return to the problem of separating two disjoint sets of points, $\{u_i\}_{i=1}^p$ and $\{v_j\}_{j=1}^q$, but this time we do not assume that these two sets are separable. To cope with nonseparability, we allow points to invade the safety zone around the separating hyperplane, and even points on the wrong side of the hyperplane. Such a method is called soft margin support vector machine. We discuss variations of this method, including $\nu$-SV classification. In each case, we present a careful derivation of the dual.

Except for a few exceptions we provide complete proofs. We did so to make this book self-contained, but also because we believe that no deep knowledge of this material can be acquired without working out some proofs. However, our advice is to skip some of the proofs upon first reading, especially if they are long and intricate.
Part I

Preliminaries for Optimization Theory
Chapter 2

Topology

2.1 Metric Spaces and Normed Vector Spaces

This chapter contains a review of basic topological concepts. First metric spaces are defined. Next normed vector spaces are defined. Closed and open sets are defined, and their basic properties are stated. The general concept of a topological space is defined. The closure and the interior of a subset are defined. The subspace topology and the product topology are defined. Continuous maps and homeomorphisms are defined. Limits of sequences are defined. Continuous linear maps and multilinear maps are defined and studied briefly. The chapter ends with the definition of a normed affine space.

Most spaces considered in this book have a topological structure given by a metric or a norm, and we first review these notions. We begin with metric spaces. Recall that \( \mathbb{R}_+ = \{ x \in \mathbb{R} \mid x \geq 0 \} \).

**Definition 2.1.** A *metric space* is a set \( E \) together with a function \( d: E \times E \to \mathbb{R}_+ \), called a *metric*, or distance, assigning a nonnegative real number \( d(x, y) \) to any two points \( x, y \in E \), and satisfying the following conditions for all \( x, y, z \in E \):

1. \( d(x, y) = d(y, x) \). (symmetry)
2. \( d(x, y) \geq 0 \), and \( d(x, y) = 0 \) iff \( x = y \). (positivity)
3. \( d(x, z) \leq d(x, y) + d(y, z) \). (triangle inequality)

Geometrically, Condition (D3) expresses the fact that in a triangle with vertices \( x, y, z \), the length of any side is bounded by the sum of the lengths of the other two sides. From (D3), we immediately get

\[
|d(x, y) - d(y, z)| \leq d(x, z).
\]

Let us give some examples of metric spaces. Recall that the *absolute value* \( |x| \) of a real number \( x \in \mathbb{R} \) is defined such that \( |x| = x \) if \( x \geq 0 \), \( |x| = -x \) if \( x < 0 \), and for a complex number \( x = a + ib \), by \( |x| = \sqrt{a^2 + b^2} \).
Example 2.1.

1. Let $E = \mathbb{R}$, and $d(x, y) = |x - y|$, the absolute value of $x - y$. This is the so-called natural metric on $\mathbb{R}$.

2. Let $E = \mathbb{R}^n$ (or $E = \mathbb{C}^n$). We have the Euclidean metric

$$d_2(x, y) = \left( |x_1 - y_1|^2 + \cdots + |x_n - y_n|^2 \right)^{\frac{1}{2}},$$

the distance between the points $(x_1, \ldots, x_n)$ and $(y_1, \ldots, y_n)$.

3. For every set $E$, we can define the discrete metric, defined such that $d(x, y) = 1$ iff $x \neq y$, and $d(x, x) = 0$.

4. For any $a, b \in \mathbb{R}$ such that $a < b$, we define the following sets:

$$[a, b] = \{ x \in \mathbb{R} \mid a \leq x \leq b \}, \quad (\text{closed interval})$$

$$(a, b) = \{ x \in \mathbb{R} \mid a < x < b \}, \quad (\text{open interval})$$

$$[a, b) = \{ x \in \mathbb{R} \mid a \leq x < b \}, \quad (\text{interval closed on the left, open on the right})$$

$$(a, b] = \{ x \in \mathbb{R} \mid a < x \leq b \}, \quad (\text{interval open on the left, closed on the right})$$

Let $E = [a, b]$, and $d(x, y) = |x - y|$. Then $([a, b], d)$ is a metric space.

We will need to define the notion of proximity in order to define convergence of limits and continuity of functions. For this, we introduce some standard “small neighborhoods.”

Definition 2.2. Given a metric space $E$ with metric $d$, for every $a \in E$, for every $\rho \in \mathbb{R}$, with $\rho > 0$, the set

$$B(a, \rho) = \{ x \in E \mid d(a, x) \leq \rho \}$$

is called the closed ball of center $a$ and radius $\rho$, the set

$$B_0(a, \rho) = \{ x \in E \mid d(a, x) < \rho \}$$

is called the open ball of center $a$ and radius $\rho$, and the set

$$S(a, \rho) = \{ x \in E \mid d(a, x) = \rho \}$$

is called the sphere of center $a$ and radius $\rho$. It should be noted that $\rho$ is finite (i.e., not $+\infty$). A subset $X$ of a metric space $E$ is bounded if there is a closed ball $B(a, \rho)$ such that $X \subseteq B(a, \rho)$.

Clearly, $B(a, \rho) = B_0(a, \rho) \cup S(a, \rho)$. 
Example 2.2.

1. In $E = \mathbb{R}$ with the distance $|x - y|$, an open ball of center $a$ and radius $\rho$ is the open interval $(a - \rho, a + \rho)$.

2. In $E = \mathbb{R}^2$ with the Euclidean metric, an open ball of center $a$ and radius $\rho$ is the set of points inside the disk of center $a$ and radius $\rho$, excluding the boundary points on the circle.

3. In $E = \mathbb{R}^3$ with the Euclidean metric, an open ball of center $a$ and radius $\rho$ is the set of points inside the sphere of center $a$ and radius $\rho$, excluding the boundary points on the sphere.

One should be aware that intuition can be misleading in forming a geometric image of a closed (or open) ball. For example, if $d$ is the discrete metric, a closed ball of center $a$ and radius $\rho < 1$ consists only of its center $a$, and a closed ball of center $a$ and radius $\rho \geq 1$ consists of the entire space!

If $E = [a, b]$, and $d(x, y) = |x - y|$, as in Example 19.1, an open ball $B_0(a, \rho)$, with $\rho < b - a$, is in fact the interval $[a, a + \rho)$, which is closed on the left.

We now consider a very important special case of metric spaces, normed vector spaces. Normed vector spaces have already been defined in Chapter 7 (Vol. I) (Definition 7.1 (Vol. I)) but for the reader’s convenience we repeat the definition.

Definition 2.3. Let $E$ be a vector space over a field $K$, where $K$ is either the field $\mathbb{R}$ of reals, or the field $\mathbb{C}$ of complex numbers. A norm on $E$ is a function $\|\| : E \to \mathbb{R}_+$, assigning a nonnegative real number $\|u\|$ to any vector $u \in E$, and satisfying the following conditions for all $x, y, z \in E$:

(N1) $\|x\| \geq 0$, and $\|x\| = 0$ iff $x = 0$. (positivity)

(N2) $\|\lambda x\| = |\lambda| \|x\|$. (homogeneity (or scaling))

(N3) $\|x + y\| \leq \|x\| + \|y\|$. (triangle inequality)

A vector space $E$ together with a norm $\|\|$ is called a normed vector space.

We showed in Chapter 7 (Vol. I), that

$$\|-x\| = \|x\|,$$

and from (N3), we get

$$\|\|x\| - \|y\|\| \leq \|x - y\|.$$

Given a normed vector space $E$, if we define $d$ such that

$$d(x, y) = \|x - y\|,$$
it is easily seen that $d$ is a metric. Thus, every normed vector space is immediately a metric space. Note that the metric associated with a norm is invariant under translation, that is,

$$d(x + u, y + u) = d(x, y).$$

For this reason, we can restrict ourselves to open or closed balls of center 0.

Examples of normed vector spaces were given in Example 7.1 (Vol. I). We repeat the most important examples.

**Example 2.3.** Let $E = \mathbb{R}^n$ (or $E = \mathbb{C}^n$). There are three standard norms. For every $(x_1, \ldots, x_n) \in E$, we have the norm $\|x\|_1$, defined such that,

$$\|x\|_1 = |x_1| + \cdots + |x_n|,$$

we have the *Euclidean norm* $\|x\|_2$, defined such that,

$$\|x\|_2 = (|x_1|^2 + \cdots + |x_n|^2)^{\frac{1}{2}},$$

and the *sup-norm* $\|x\|_\infty$, defined such that,

$$\|x\|_\infty = \max\{|x_i| \mid 1 \leq i \leq n\}.$$ 

More generally, we define the $\ell_p$-norm (for $p \geq 1$) by

$$\|x\|_p = (|x_1|^p + \cdots + |x_n|^p)^{1/p}.$$ 

We proved in Proposition 7.1 (Vol. I) that the $\ell_p$-norms are indeed norms. The closed unit balls centered at $(0, 0)$ for $\|\|_1$, $\|\|_2$, and $\|\|_\infty$, along with the containment relationships, are shown in Figures 19.1 and 19.2. Figures 19.3 and 19.4 illustrate the situation in $\mathbb{R}^3$. 

Figure 2.1: Figure (a) shows the diamond shaped closed ball associated with $\|\|_1$. Figure (b) shows the closed unit disk associated with $\|\|_2$, while Figure (c) illustrates the closed unit ball associated with $\|\|_\infty$. 

2.1. METRIC SPACES AND NORMED VECTOR SPACES

Figure 2.2: The relationship between the closed unit balls centered at (0, 0).

Figure 2.4: The relationship between the closed unit balls centered at (0, 0, 0).

In a normed vector space, we define a closed ball or an open ball of radius $\rho$ as a closed ball or an open ball of center 0. We may use the notation $B(\rho)$ and $B_0(\rho)$.

We will now define the crucial notions of open sets and closed sets, and of a topological space.

**Definition 2.4.** Let $E$ be a metric space with metric $d$. A subset $U \subseteq E$ is an open set in $E$ if either $U = \emptyset$, or for every $a \in U$, there is some open ball $B_0(a, \rho)$ such that, $B_0(a, \rho) \subseteq U$.

A subset $F \subseteq E$ is a closed set in $E$ if its complement $E - F$ is open in $E$. See Figure 19.5.

The set $E$ itself is open, since for every $a \in E$, every open ball of center $a$ is contained in $E$. In $E = \mathbb{R}^n$, given $n$ intervals $[a_i, b_i]$, with $a_i < b_i$, it is easy to show that the open $n$-cube

$$\{(x_1, \ldots, x_n) \in E \mid a_i < x_i < b_i, \ 1 \leq i \leq n\}$$

is an open set. In fact, it is possible to find a metric for which such open $n$-cubes are open balls! Similarly, we can define the closed $n$-cube

$$\{(x_1, \ldots, x_n) \in E \mid a_i \leq x_i \leq b_i, \ 1 \leq i \leq n\},$$

Recall that $\rho > 0$.\footnote{Recall that $\rho > 0$.}
which is a closed set.

The open sets satisfy some important properties that lead to the definition of a topological space.

**Proposition 2.1.** Given a metric space $E$ with metric $d$, the family $\mathcal{O}$ of all open sets defined in Definition 19.4 satisfies the following properties:

(O1) For every finite family $(U_i)_{1 \leq i \leq n}$ of sets $U_i \in \mathcal{O}$, we have $U_1 \cap \cdots \cap U_n \in \mathcal{O}$, i.e., $\mathcal{O}$ is closed under finite intersections.

(O2) For every arbitrary family $(U_i)_{i \in I}$ of sets $U_i \in \mathcal{O}$, we have $\bigcup_{i \in I} U_i \in \mathcal{O}$, i.e., $\mathcal{O}$ is closed under arbitrary unions.

(O3) $\emptyset \in \mathcal{O}$, and $E \in \mathcal{O}$, i.e., $\emptyset$ and $E$ belong to $\mathcal{O}$.

Furthermore, for any two distinct points $a \neq b$ in $E$, there exist two open sets $U_a$ and $U_b$ such that, $a \in U_a$, $b \in U_b$, and $U_a \cap U_b = \emptyset$. 
2.2. TOPOLOGICAL SPACES

Figure 2.5: An open set $U$ in $E = \mathbb{R}^2$ under the standard Euclidean metric. Any point in the peach set $U$ is surrounded by a small raspberry open set which lies within $U$.

Proof. It is straightforward. For the last point, letting $\rho = d(a, b)/3$ (in fact $\rho = d(a, b)/2$ works too), we can pick $U_a = B_0(a, \rho)$ and $U_b = B_0(b, \rho)$. By the triangle inequality, we must have $U_a \cap U_b = \emptyset$. \hfill $\blacksquare$

The above proposition leads to the very general concept of a topological space.

One should be careful that, in general, the family of open sets is not closed under infinite intersections. For example, in $\mathbb{R}$ under the metric $|x - y|$, letting $U_n = (-1/n, +1/n)$, each $U_n$ is open, but $\bigcap_n U_n = \{0\}$, which is not open.

2.2 Topological Spaces

Motivated by Proposition 19.1, a topological space is defined in terms of a family of sets satisfying the properties of open sets stated in that proposition.

Definition 2.5. Given a set $E$, a topology on $E$ (or a topological structure on $E$), is defined as a family $\mathcal{O}$ of subsets of $E$ called open sets, and satisfying the following three properties:

1. For every finite family $(U_i)_{1 \leq i \leq n}$ of sets $U_i \in \mathcal{O}$, we have $U_1 \cap \cdots \cap U_n \in \mathcal{O}$, i.e., $\mathcal{O}$ is closed under finite intersections.

2. For every arbitrary family $(U_i)_{i \in I}$ of sets $U_i \in \mathcal{O}$, we have $\bigcup_{i \in I} U_i \in \mathcal{O}$, i.e., $\mathcal{O}$ is closed under arbitrary unions.

3. $\emptyset \in \mathcal{O}$, and $E \in \mathcal{O}$, i.e., $\emptyset$ and $E$ belong to $\mathcal{O}$.

A set $E$ together with a topology $\mathcal{O}$ on $E$ is called a topological space. Given a topological space $(E, \mathcal{O})$, a subset $F$ of $E$ is a closed set if $F = E - U$ for some open set $U \in \mathcal{O}$, i.e., $F$ is the complement of some open set.
It is possible that an open set is also a closed set. For example, $\emptyset$ and $E$ are both open and closed. When a topological space contains a proper nonempty subset $U$ which is both open and closed, the space $E$ is said to be disconnected.

A topological space $(E, \mathcal{O})$ is said to satisfy the Hausdorff separation axiom (or $T_2$-separation axiom) if for any two distinct points $a \neq b$ in $E$, there exist two open sets $U_a$ and $U_b$ such that, $a \in U_a$, $b \in U_b$, and $U_a \cap U_b = \emptyset$. When the $T_2$-separation axiom is satisfied, we also say that $(E, \mathcal{O})$ is a Hausdorff space.

As shown by Proposition 19.1, any metric space is a topological Hausdorff space, the family of open sets being in fact the family of arbitrary unions of open balls. Similarly, any normed vector space is a topological Hausdorff space, the family of open sets being the family of arbitrary unions of open balls. The topology $\mathcal{O}$ consisting of all subsets of $E$ is called the discrete topology.

Remark: Most (if not all) spaces used in analysis are Hausdorff spaces. Intuitively, the Hausdorff separation axiom says that there are enough “small” open sets. Without this axiom, some counter-intuitive behaviors may arise. For example, a sequence may have more than one limit point (or a compact set may not be closed). Nevertheless, non-Hausdorff topological spaces arise naturally in algebraic geometry. But even there, some substitute for separation is used.

One of the reasons why topological spaces are important is that the definition of a topology only involves a certain family $\mathcal{O}$ of sets, and not how such family is generated from a metric or a norm. For example, different metrics or different norms can define the same family of open sets. Many topological properties only depend on the family $\mathcal{O}$ and not on the specific metric or norm. But the fact that a topology is definable from a metric or a norm is important, because it usually implies nice properties of a space. All our examples will be spaces whose topology is defined by a metric or a norm.

By taking complements, we can state properties of the closed sets dual to those of Definition 19.5. Thus, $\emptyset$ and $E$ are closed sets, and the closed sets are closed under finite unions and arbitrary intersections.

It is also worth noting that the Hausdorff separation axiom implies that for every $a \in E$, the set $\{a\}$ is closed. Indeed, if $x \in E - \{a\}$, then $x \neq a$, and so there exist open sets $U_a$ and $U_x$ such that $a \in U_a$, $x \in U_x$, and $U_a \cap U_x = \emptyset$. See Figure 19.6. Thus, for every $x \in E - \{a\}$, there is an open set $U_x$ containing $x$ and contained in $E - \{a\}$, showing by (O3) that $E - \{a\}$ is open, and thus that the set $\{a\}$ is closed.

Given a topological space $(E, \mathcal{O})$, given any subset $A$ of $E$, since $E \in \mathcal{O}$ and $E$ is a closed set, the family $\mathcal{C}_A = \{F \mid A \subseteq F, F \text{ a closed set}\}$ of closed sets containing $A$ is nonempty, and since any arbitrary intersection of closed sets is a closed set, the intersection $\bigcap \mathcal{C}_A$ of the sets in the family $\mathcal{C}_A$ is the smallest closed set containing $A$. By a similar reasoning, the union of all the open subsets contained in $A$ is the largest open set contained in $A$. 
Definition 2.6. Given a topological space \((E, \mathcal{O})\), given any subset \(A\) of \(E\), the smallest closed set containing \(A\) is denoted by \(\overline{A}\), and is called the closure, or adherence of \(A\). See Figure 19.7. A subset \(A\) of \(E\) is dense in \(E\) if \(\overline{A} = E\). The largest open set contained in \(A\) is denoted by \(\mathring{A}\), and is called the interior of \(A\). See Figure 19.8. The set \(\text{Fr} A = \overline{A} \cap E - A\) is called the boundary (or frontier) of \(A\). We also denote the boundary of \(A\) by \(\partial A\). See Figure 19.9.
Figure 2.8: The topological space \((E, \mathcal{O})\) is \(\mathbb{R}^2\) with topology induced by the Euclidean metric. The subset \(A\) is the section \(B_0(1)\) in the first and fourth quadrants bound by the lines \(y = x\) and \(y = -x\). The interior of \(A\) is obtained by the covering \(A\) with small open balls.

Figure 2.9: The topological space \((E, \mathcal{O})\) is \(\mathbb{R}^2\) with topology induced by the Euclidean metric. The subset \(A\) is the section \(B_0(1)\) in the first and fourth quadrants bound by the lines \(y = x\) and \(y = -x\). The boundary of \(A\) is \(\bar{A} \setminus \overset{o}{A}\).

**Remark:** The notation \(\bar{A}\) for the closure of a subset \(A\) of \(E\) is somewhat unfortunate, since \(\bar{A}\) is often used to denote the set complement of \(A\) in \(E\). Still, we prefer it to more cumbersome notations such as \(\text{clo}(A)\), and we denote the complement of \(A\) in \(E\) by \(E \setminus A\) (or sometimes, \(A^c\)).

By definition, it is clear that a subset \(A\) of \(E\) is closed iff \(A = \bar{A}\). The set \(\mathbb{Q}\) of rationals is dense in \(\mathbb{R}\). It is easily shown that \(\bar{A} = \overset{\circ}{A} \cup \partial A\) and \(\overset{\circ}{A} \cap \partial A = \emptyset\). Another useful characterization of \(\bar{A}\) is given by the following proposition.
Proposition 2.2. Given a topological space $(E, \mathcal{O})$, given any subset $A$ of $E$, the closure $\overline{A}$ of $A$ is the set of all points $x \in E$ such that for every open set $U$ containing $x$, then $U \cap A \neq \emptyset$. See Figure 19.10.

Figure 2.10: The topological space $(E, \mathcal{O})$ is $\mathbb{R}^2$ with topology induced by the Euclidean metric. The purple subset $A$ is illustrated with three red points, each in its closure since the open ball centered at each point has nontrivial intersection with $A$.

Proof. If $A = \emptyset$, since $\emptyset$ is closed, the proposition holds trivially. Thus, assume that $A \neq \emptyset$. First, assume that $x \in \overline{A}$. Let $U$ be any open set such that $x \in U$. If $U \cap A = \emptyset$, since $U$ is open, then $E - U$ is a closed set containing $A$, and since $\overline{A}$ is the intersection of all closed sets containing $A$, we must have $x \in E - U$, which is impossible. Conversely, assume that $x \in E$ is a point such that for every open set $U$ containing $x$, then $U \cap A \neq \emptyset$. Let $F$ be any closed subset containing $A$. If $x \notin F$, since $F$ is closed, then $U = E - F$ is an open set such that $x \in U$, and $U \cap A = \emptyset$, a contradiction. Thus, we have $x \in F$ for every closed set containing $A$, that is, $x \in \overline{A}$. \qed

Often, it is necessary to consider a subset $A$ of a topological space $E$, and to view the subset $A$ as a topological space. The following proposition shows how to define a topology on a subset.

Proposition 2.3. Given a topological space $(E, \mathcal{O})$, given any subset $A$ of $E$, let

$$U = \{ U \cap A \mid U \in \mathcal{O} \}$$

be the family of all subsets of $A$ obtained as the intersection of any open set in $\mathcal{O}$ with $A$. The following properties hold.
(1) The space \((A, \mathcal{U})\) is a topological space.

(2) If \(E\) is a metric space with metric \(d\), then the restriction \(d_A: A \times A \to \mathbb{R}_+\) of the metric \(d\) to \(A\) defines a metric space. Furthermore, the topology induced by the metric \(d_A\) agrees with the topology defined by \(\mathcal{U}\), as above.

Proof. Left as an exercise. \(\square\)

Proposition 19.3 suggests the following definition.

Definition 2.7. Given a topological space \((E, \mathcal{O})\), given any subset \(A\) of \(E\), the subpace topology on \(A\) induced by \(\mathcal{O}\) is the family \(\mathcal{U}\) of open sets defined such that

\[
\mathcal{U} = \{U \cap A \mid U \in \mathcal{O}\}
\]

is the family of all subsets of \(A\) obtained as the intersection of any open set in \(\mathcal{O}\) with \(A\). We say that \((A, \mathcal{U})\) has the subpace topology. If \((E, d)\) is a metric space, the restriction \(d_A: A \times A \to \mathbb{R}_+\) of the metric \(d\) to \(A\) is called the subpace metric.

For example, if \(E = \mathbb{R}^n\) and \(d\) is the Euclidean metric, we obtain the subpace topology on the closed \(n\)-cube

\[
\{(x_1, \ldots, x_n) \in E \mid a_i \leq x_i \leq b_i, 1 \leq i \leq n\}.
\]

See Figure 19.11.

One should realize that every open set \(U \in \mathcal{O}\) which is entirely contained in \(A\) is also in the family \(\mathcal{U}\), but \(\mathcal{U}\) may contain open sets that are not in \(\mathcal{O}\). For example, if \(E = \mathbb{R}\) with \(|x - y|\), and \(A = [a, b]\), then sets of the form \([a, c]\), with \(a < c < b\) belong to \(\mathcal{U}\), but they are not open sets for \(\mathbb{R}\) under \(|x - y|\). However, there is agreement in the following situation.

Proposition 2.4. Given a topological space \((E, \mathcal{O})\), given any subset \(A\) of \(E\), if \(\mathcal{U}\) is the subpace topology, then the following properties hold.

(1) If \(A\) is an open set \(A \in \mathcal{O}\), then every open set \(U \in \mathcal{U}\) is an open set \(U \in \mathcal{O}\).

(2) If \(A\) is a closed set in \(E\), then every closed set w.r.t. the subpace topology is a closed set w.r.t. \(\mathcal{O}\).

Proof. Left as an exercise. \(\square\)

The concept of product topology is also useful. We have the following proposition.

Proposition 2.5. Given \(n\) topological spaces \((E_i, \mathcal{O}_i)\), let \(\mathcal{B}\) be the family of subsets of \(E_1 \times \cdots \times E_n\) defined as follows:

\[
\mathcal{B} = \{U_1 \times \cdots \times U_n \mid U_i \in \mathcal{O}_i, 1 \leq i \leq n\},
\]

and let \(\mathcal{P}\) be the family consisting of arbitrary unions of sets in \(\mathcal{B}\), including \(\emptyset\). Then, \(\mathcal{P}\) is a topology on \(E_1 \times \cdots \times E_n\).
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Figure 2.11: An example of an open set in the subspace topology for \( \{(x, y, z) \in \mathbb{R}^3 \mid -1 \leq x \leq 1, -1 \leq y \leq 1, -1 \leq z \leq 1\} \). The open set is the corner region \( ABCD \) and is obtained by intersection the cube \( B_0((1, 1, 1), 1) \).

Proof. Left as an exercise.

Definition 2.8. Given \( n \) topological spaces \( (E_i, O_i) \), the product topology on \( E_1 \times \cdots \times E_n \) is the family \( \mathcal{P} \) of subsets of \( E_1 \times \cdots \times E_n \) defined as follows: if

\[
\mathcal{B} = \left\{ U_1 \times \cdots \times U_n \mid U_i \in O_i, 1 \leq i \leq n \right\},
\]

then \( \mathcal{P} \) is the family consisting of arbitrary unions of sets in \( \mathcal{B} \), including \( \emptyset \). See Figure 19.12.

If each \( (E_i, d_{E_i}) \) is a metric space, there are three natural metrics that can be defined on \( E_1 \times \cdots \times E_n \):

\[
d_1((x_1, \ldots, x_n), (y_1, \ldots, y_n)) = d_{E_1}(x_1, y_1) + \cdots + d_{E_n}(x_n, y_n),
\]

\[
d_2((x_1, \ldots, x_n), (y_1, \ldots, y_n)) = \left( (d_{E_1}(x_1, y_1))^2 + \cdots + (d_{E_n}(x_n, y_n))^2 \right)^{\frac{1}{2}},
\]

\[
d_\infty((x_1, \ldots, x_n), (y_1, \ldots, y_n)) = \max\{d_{E_1}(x_1, y_1), \ldots, d_{E_n}(x_n, y_n)\}.
\]
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Figure 2.12: Examples of open sets in the product topology for \( \mathbb{R}^2 \) and \( \mathbb{R}^3 \) induced by the Euclidean metric.

It is easy to show that
\[
d_{\infty}((x_1, \ldots, x_n), (y_1, \ldots, y_n)) \leq d_2((x_1, \ldots, x_n), (y_1, \ldots, y_n)) \leq d_1((x_1, \ldots, x_n), (y_1, \ldots, y_n)) \leq nd_{\infty}((x_1, \ldots, x_n), (y_1, \ldots, y_n)),
\]
so these distances define the same topology, which is the product topology.

If each \((E_i, ||\cdot||_{E_i})\) is a normed vector space, there are three natural norms that can be defined on \(E_1 \times \cdots \times E_n\):
\[
||(x_1, \ldots, x_n)||_1 = ||x_1||_{E_1} + \cdots + ||x_n||_{E_n},
||(x_1, \ldots, x_n)||_2 = \left(||x_1||^2_{E_1} + \cdots + ||x_n||^2_{E_n}\right)^{\frac{1}{2}},
||(x_1, \ldots, x_n)||_{\infty} = \max\{||x_1||_{E_1}, \ldots, ||x_n||_{E_n}\}.
\]

It is easy to show that
\[
||(x_1, \ldots, x_n)||_{\infty} \leq ||(x_1, \ldots, x_n)||_2 \leq ||(x_1, \ldots, x_n)||_1 \leq n ||(x_1, \ldots, x_n)||_{\infty},
\]
so these norms define the same topology, which is the product topology. It can also be verified that when \(E_i = \mathbb{R}\), with the standard topology induced by \(|x - y|\), the topology product on \(\mathbb{R}^n\) is the standard topology induced by the Euclidean norm.

**Definition 2.9.** Two metrics \(d_1\) and \(d_2\) on a space \(E\) are equivalent if they induce the same topology \(\mathcal{O}\) on \(E\) (i.e., they define the same family \(\mathcal{O}\) of open sets). Similarly, two norms \(||\cdot||_1\) and \(||\cdot||_2\) on a space \(E\) are equivalent if they induce the same topology \(\mathcal{O}\) on \(E\).

**Remark:** Given a topological space \((E, \mathcal{O})\), it is often useful, as in Proposition 19.5, to define the topology \(\mathcal{O}\) in terms of a subfamily \(\mathcal{B}\) of subsets of \(E\). We say that a family \(\mathcal{B}\) of
2.2. TOPOLOGICAL SPACES

subsets of $E$ is a basis for the topology $\mathcal{O}$, if $\mathcal{B}$ is a subset of $\mathcal{O}$, and if every open set $U$ in $\mathcal{O}$ can be obtained as some union (possibly infinite) of sets in $\mathcal{B}$ (agreeing that the empty union is the empty set).

For example, given any metric space $(E, d)$, $\mathcal{B} = \{ B_\rho(a, \rho) \mid a \in E, \rho > 0 \}$. In particular, if $d = \| \|_2$, the open intervals form a basis for $\mathbb{R}$, while the open disks form a basis for $\mathbb{R}^2$. The open rectangles also form a basis for $\mathbb{R}^2$ with the standard topology. See Figure 19.13.

It is immediately verified that if a family $\mathcal{B} = (U_i)_{i \in I}$ is a basis for the topology of $(E, \mathcal{O})$, then $E = \bigcup_{i \in I} U_i$, and the intersection of any two sets $U_i, U_j \in \mathcal{B}$ is the union of some sets in the family $\mathcal{B}$ (again, agreeing that the empty union is the empty set). Conversely, a family $\mathcal{B}$ with these properties is the basis of the topology obtained by forming arbitrary unions of sets in $\mathcal{B}$.

A subbasis for $\mathcal{O}$ is a family $\mathcal{S}$ of subsets of $E$, such that the family $\mathcal{B}$ of all finite intersections of sets in $\mathcal{S}$ (including $E$ itself, in case of the empty intersection) is a basis of $\mathcal{O}$. See Figure 19.13

![Figure 2.13: Figure (i.) shows that the set of infinite open intervals forms a subbasis for $\mathbb{R}$. Figure (ii.) shows that the infinite open strips form a subbasis for $\mathbb{R}^2$.](image)

The following proposition gives useful criteria for determining whether a family of open subsets is a basis of a topological space.

**Proposition 2.6.** Given a topological space $(E, \mathcal{O})$ and a family $\mathcal{B}$ of open subsets in $\mathcal{O}$ the following properties hold:

1. The family $\mathcal{B}$ is a basis for the topology $\mathcal{O}$ iff for every open set $U \in \mathcal{O}$ and every $x \in U$, there is some $B \in \mathcal{B}$ such that $x \in B$ and $B \subseteq U$. See Figure 19.14.

2. The family $\mathcal{B}$ is a basis for the topology $\mathcal{O}$ iff
   
   (a) For every $x \in E$, there is some $B \in \mathcal{B}$ such that $x \in B$. 


(b) For any two open subsets, $B_1, B_2 \in \mathcal{B}$, for every $x \in E$, if $x \in B_1 \cap B_2$, then there is some $B_3 \in \mathcal{B}$ such that $x \in B_3$ and $B_3 \subseteq B_1 \cap B_2$. See Figure 19.15.

Figure 2.14: Given an open subset $U$ of $\mathbb{R}^2$ and $x \in U$, there exists an open ball $B$ containing $x$ with $B \subset U$. There also exists an open rectangle $B_1$ containing $x$ with $B_1 \subset U$.

Figure 2.15: A schematic illustration of Condition (b) in Proposition 19.6.

We now consider the fundamental property of continuity.

### 2.3 Continuous Functions, Limits

**Definition 2.10.** Let $(E, \mathcal{O}_E)$ and $(F, \mathcal{O}_F)$ be topological spaces, and let $f: E \to F$ be a function. For every $a \in E$, we say that $f$ is continuous at $a$, if for every open set $V \in \mathcal{O}_F$ containing $f(a)$, there is some open set $U \in \mathcal{O}_E$ containing $a$, such that, $f(U) \subseteq V$. See Figure 19.16. We say that $f$ is continuous if it is continuous at every $a \in E$.

Define a neighborhood of $a \in E$ as any subset $N$ of $E$ containing some open set $O \in \mathcal{O}$ such that $a \in O$. Now, if $f$ is continuous at $a$ and $N$ is any neighborhood of $f(a)$, there is some open set $V \subseteq N$ containing $f(a)$, and since $f$ is continuous at $a$, there is some open
set $U$ containing $a$, such that $f(U) \subseteq V$. Since $V \subseteq N$, the open set $U$ is a subset of $f^{-1}(N)$ containing $a$, and $f^{-1}(N)$ is a neighborhood of $a$. Conversely, if $f^{-1}(N)$ is a neighborhood of $a$ whenever $N$ is any neighborhood of $f(a)$, it is immediate that $f$ is continuous at $a$. See Figure 19.17.

![Figure 2.16: A schematic illustration of Definition 19.10.](image1)

![Figure 2.17: A schematic illustration of the neighborhood condition.](image2)

It is easy to see that Definition 19.10 is equivalent to the following statements.

**Proposition 2.7.** Let $(E, \mathcal{O}_E)$ and $(F, \mathcal{O}_F)$ be topological spaces, and let $f: E \rightarrow F$ be a function. For every $a \in E$, the function $f$ is continuous at $a \in E$ iff for every neighborhood $N$ of $f(a) \in F$, then $f^{-1}(N)$ is a neighborhood of $a$. The function $f$ is continuous on $E$ iff $f^{-1}(V)$ is an open set in $\mathcal{O}_E$ for every open set $V \in \mathcal{O}_F$.

If $E$ and $F$ are metric spaces defined by metrics $d_1$ and $d_2$, we can show easily that $f$ is continuous at $a$ iff

for every $\epsilon > 0$, there is some $\eta > 0$, such that, for every $x \in E$,

$$
\text{if } d_1(a, x) \leq \eta, \text{ then } d_2(f(a), f(x)) \leq \epsilon.
$$

Similarly, if $E$ and $F$ are normed vector spaces defined by norms $\| \cdot \|_1$ and $\| \cdot \|_2$, we can show easily that $f$ is continuous at $a$ iff
for every $\epsilon > 0$, there is some $\eta > 0$, such that, for every $x \in E$,
\[
\text{if } \|x - a\|_1 \leq \eta, \text{ then } \|f(x) - f(a)\|_2 \leq \epsilon.
\]

It is worth noting that continuity is a topological notion, in the sense that equivalent metrics (or equivalent norms) define exactly the same notion of continuity.

If $(E, \mathcal{O}_E)$ and $(F, \mathcal{O}_F)$ are topological spaces, and $f: E \to F$ is a function, for every nonempty subset $A \subseteq E$ of $E$, we say that $f$ is continuous on $A$ if the restriction of $f$ to $A$ is continuous with respect to $(A, \mathcal{U})$ and $(F, \mathcal{O}_F)$, where $\mathcal{U}$ is the subspace topology induced by $\mathcal{O}_E$ on $A$.

Given a product $E_1 \times \cdots \times E_n$ of topological spaces, as usual, we let $\pi_i: E_1 \times \cdots \times E_n \to E_i$ be the projection function such that, $\pi_i(x_1, \ldots, x_n) = x_i$. It is immediately verified that each $\pi_i$ is continuous.

Given a topological space $(E, \mathcal{O})$, we say that a point $a \in E$ is isolated if $\{a\}$ is an open set in $\mathcal{O}$. Then if $(E, \mathcal{O}_E)$ and $(F, \mathcal{O}_F)$ are topological spaces, any function $f: E \to F$ is continuous at every isolated point $a \in E$. In the discrete topology, every point is isolated.

In a nontrivial normed vector space $(E, \|\|)$ (with $E \neq \{0\}$), no point is isolated. To show this, we show that every open ball $B_0(u, \rho)$ contains some vectors different from $u$. Indeed, since $E$ is nontrivial, there is some $v \in E$ such that $v \neq 0$, and thus $\lambda = \|v\| > 0$ (by (N1)). Let
\[
w = u + \frac{\rho}{\lambda + 1}v.
\]
Since $v \neq 0$ and $\rho > 0$, we have $w \neq u$. Then,
\[
\|w - u\| = \left\| \frac{\rho}{\lambda + 1}v \right\| = \frac{\rho \lambda}{\lambda + 1} < \rho,
\]
which shows that $\|w - u\| < \rho$, for $w \neq u$.

The following proposition is easily shown.

**Proposition 2.8.** Given topological spaces $(E, \mathcal{O}_E)$, $(F, \mathcal{O}_F)$, and $(G, \mathcal{O}_G)$, and two functions $f: E \to F$ and $g: F \to G$, if $f$ is continuous at $a \in E$ and $g$ is continuous at $f(a) \in F$, then $g \circ f: E \to G$ is continuous at $a \in E$. Given $n$ topological spaces $(F_i, \mathcal{O}_i)$, for every function $f: E \to F_1 \times \cdots \times F_n$, then $f$ is continuous at $a \in E$ iff every $f_i: E \to F_i$ is continuous at $a$, where $f_i = \pi_i \circ f$.

One can also show that in a metric space $(E, d)$, the distance $d: E \times E \to \mathbb{R}$ is continuous, where $E \times E$ has the product topology. By the triangle inequality, we have
\[
d(x, y) \leq d(x, x_0) + d(x_0, y_0) + d(y_0, y) = d(x_0, y_0) + d(x_0, x) + d(y_0, y)
\]
and
\[
d(x_0, y_0) \leq d(x_0, x) + d(x, y) + d(y, y_0) = d(x, y) + d(x_0, x) + d(y_0, y).
\]
Consequently,
\[ |d(x, y) - d(x_0, y_0)| \leq d(x_0, x) + d(y_0, y), \]
which proves that \( d \) is continuous at \((x_0, y_0)\). In fact this shows that \( d \) is uniformly continuous; see Definition 19.14.

Similarly, for a normed vector space \((E, \| \|)\), the norm \( \| \|: E \to \mathbb{R} \) is (uniformly) continuous.

Given a function \( f: E_1 \times \cdots \times E_n \to F \), we can fix \( n-1 \) of the arguments, say \( a_1, \ldots, a_{i-1}, a_{i+1}, \ldots, a_n \), and view \( f \) as a function of the remaining argument,
\[
x_i \mapsto f(a_1, \ldots, a_{i-1}, x_i, a_{i+1}, \ldots, a_n),
\]
where \( x_i \in E_i \). If \( f \) is continuous, it is clear that each \( f_i \) is continuous.

One should be careful that the converse is false! For example, consider the function \( f: \mathbb{R} \times \mathbb{R} \to \mathbb{R} \), defined such that,
\[
f(x, y) = \frac{xy}{x^2 + y^2} \quad \text{if} \ (x, y) \neq (0, 0), \quad \text{and} \quad f(0, 0) = 0.
\]
The function \( f \) is continuous on \( \mathbb{R} \times \mathbb{R} - \{(0, 0)\} \), but on the line \( y = mx \), with \( m \neq 0 \), we have \( f(x, y) = \frac{m}{1+m^2} \neq 0 \), and thus, on this line, \( f(x, y) \) does not approach 0 when \((x, y)\) approaches \((0,0)\). See Figure 19.18.

![Figure 2.18: The graph of \( f(x, y) = \frac{xy}{x^2 + y^2} \) for \((x, y) \neq (0,0)\). The bottom of this graph, which shows the approach along the line \( y = -x \), does not have a \( z \) value of 0.](image)

The following proposition is useful for showing that real-valued functions are continuous.

**Proposition 2.9.** If \( E \) is a topological space, and \((\mathbb{R}, |x - y|)\) the reals under the standard topology, for any two functions \( f: E \to \mathbb{R} \) and \( g: E \to \mathbb{R} \), for any \( a \in E \), for any \( \lambda \in \mathbb{R} \), if \( f \) and \( g \) are continuous at \( a \), then \( f + g \), \( \lambda f \), \( f \cdot g \), are continuous at \( a \), and \( f/g \) is continuous at \( a \) if \( g(a) \neq 0 \).
Proof. Left as an exercise.

Using Proposition 19.9, we can show easily that every real polynomial function is continuous.

The notion of isomorphism of topological spaces is defined as follows.

**Definition 2.11.** Let \((E, \mathcal{O}_E)\) and \((F, \mathcal{O}_F)\) be topological spaces, and let \(f: E \to F\) be a function. We say that \(f\) is a **homeomorphism between** \(E\) and \(F\) if \(f\) is bijective, and both \(f: E \to F\) and \(f^{-1}: F \to E\) are continuous.

One should be careful that a bijective continuous function \(f: E \to F\) is not necessarily a homeomorphism. For example, if \(E = \mathbb{R}\) with the discrete topology, and \(F = \mathbb{R}\) with the standard topology, the identity is not a homeomorphism. Another interesting example involving a parametric curve is given below. Let \(L: \mathbb{R} \to \mathbb{R}^2\) be the function, defined such that,

\[
L_1(t) = \frac{t(1 + t^2)}{1 + t^4}, \\
L_2(t) = \frac{t(1 - t^2)}{1 + t^4}.
\]

If we think of \((x(t), y(t)) = (L_1(t), L_2(t))\) as a geometric point in \(\mathbb{R}^2\), the set of points \((x(t), y(t))\) obtained by letting \(t\) vary in \(\mathbb{R}\) from \(-\infty\) to \(+\infty\), defines a curve having the shape of a “figure eight”, with self-intersection at the origin, called the “lemniscate of Bernoulli”. See Figure 19.19. The map \(L\) is continuous, and in fact bijective, but its inverse \(L^{-1}\) is not continuous. Indeed, when we approach the origin on the branch of the curve in the upper left quadrant (i.e., points such that, \(x \leq 0, y \geq 0\)), then \(t\) goes to \(-\infty\), and when we approach the origin on the branch of the curve in the lower right quadrant (i.e., points such that, \(x \geq 0, y \leq 0\)), then \(t\) goes to \(+\infty\).

![Figure 2.19: The lemniscate of Bernoulli](image)

We also review the concept of limit of a sequence. Given any set \(E\), a **sequence** is any function \(x: \mathbb{N} \to E\), usually denoted by \((x_n)_{n \in \mathbb{N}}\), or \((x_n)_{n \geq 0}\), or even by \((x_n)\).
### Definition 2.12
Given a topological space \((E, \mathcal{O})\), we say that a sequence \((x_n)_{n \in \mathbb{N}}\) converges to some \(a \in E\) if for every open set \(U\) containing \(a\), there is some \(n_0 \geq 0\), such that, \(x_n \in U\), for all \(n \geq n_0\). We also say that \(a\) is a limit of \((x_n)_{n \in \mathbb{N}}\). See Figure 19.20.

When \(E\) is a metric space with metric \(d\), it is easy to show that this is equivalent to the fact that,

for every \(\epsilon > 0\), there is some \(n_0 \geq 0\), such that, \(d(x_n, a) \leq \epsilon\), for all \(n \geq n_0\).

When \(E\) is a normed vector space with norm \(\|\|\), it is easy to show that this is equivalent to the fact that,

for every \(\epsilon > 0\), there is some \(n_0 \geq 0\), such that, \(\|x_n - a\| \leq \epsilon\), for all \(n \geq n_0\).

The following proposition shows the importance of the Hausdorff separation axiom.

### Proposition 2.10
Given a topological space \((E, \mathcal{O})\), if the Hausdorff separation axiom holds, then every sequence has at most one limit.

**Proof.** Left as an exercise. \(\square\)

It is worth noting that the notion of limit is topological, in the sense that a sequence converge to a limit \(b\) iff it converges to the same limit \(b\) in any equivalent metric (and similarly for equivalent norms).

If \(E\) is a metric space and if \(A\) is a subset of \(E\), there is a convenient way of showing that a point \(x \in E\) belongs to the closure \(\overline{A}\) of \(A\) in terms of sequences.

### Proposition 2.11
Given any metric space \((E, d)\), for any subset \(A\) of \(E\) and any point \(x \in E\), we have \(x \in \overline{A}\) iff there is a sequence \((a_n)\) of points \(a_n \in A\) converging to \(x\).
Proof. If the sequence \((a_n)\) of points \(a_n \in A\) converges to \(x\), then for every open subset \(U\) of \(E\) containing \(x\), there is some \(n_0\) such that \(a_n \in U\) for all \(n \geq n_0\), so \(U \cap A \neq \emptyset\), and Proposition 19.2 implies that \(x \in \overline{A}\).

Conversely, assume that \(x \in \overline{A}\). Then for every \(n \geq 1\), consider the open ball \(B_0(x, 1/n)\). By Proposition 19.2, we have \(B_0(x, 1/n) \cap A \neq \emptyset\), so we can pick some \(a_n \in B_0(x, 1/n) \cap A\). This way, we define a sequence \((a_n)\) of points in \(A\), and by construction \(d(x, a_n) < 1/n\) for all \(n \geq 1\), so the sequence \((a_n)\) converges to \(x\).

We still need one more concept of limit for functions.

**Definition 2.13.** Let \((E, \mathcal{O}_E)\) and \((F, \mathcal{O}_F)\) be topological spaces, let \(A\) be some nonempty subset of \(E\), and let \(f: A \to F\) be a function. For any \(a \in A\) and any \(b \in F\), we say that \(f(x)\) approaches \(b\) as \(x\) approaches \(a\) with values in \(A\) if for every open set \(V \in \mathcal{O}_F\) containing \(b\), there is some open set \(U \in \mathcal{O}_E\) containing \(a\), such that, \(f(U \cap A) \subseteq V\). See Figure 19.21. This is denoted by

\[
\lim_{x \to a, x \in A} f(x) = b.
\]

![Figure 2.21: A schematic illustration of Definition 19.13.](image-url)

First, note that by Proposition 19.2, since \(a \in \overline{A}\), for every open set \(U\) containing \(a\), we have \(U \cap A \neq \emptyset\), and the definition is nontrivial. Also, even if \(a \in A\), the value \(f(a)\) of \(f\) at \(a\) plays no role in this definition. When \(E\) and \(F\) are metric space with metrics \(d_1\) and \(d_2\), it can be shown easily that the definition can be stated as follows:

For every \(\epsilon > 0\), there is some \(\eta > 0\), such that, for every \(x \in A\),

\[
\text{if } d_1(x, a) \leq \eta, \text{ then } d_2(f(x), b) \leq \epsilon.
\]

When \(E\) and \(F\) are normed vector spaces with norms \(||\cdot||_1\) and \(||\cdot||_2\), it can be shown easily that the definition can be stated as follows:
For every $\epsilon > 0$, there is some $\eta > 0$, such that, for every $x \in A$,

$$\text{if } \|x - a\|_1 \leq \eta, \text{ then } \|f(x) - b\|_2 \leq \epsilon.$$ 

We have the following result relating continuity at a point and the previous notion.

**Proposition 2.12.** Let $(E, O_E)$ and $(F, O_F)$ be two topological spaces, and let $f : E \to F$ be a function. For any $a \in E$, the function $f$ is continuous at $a$ iff $f(x)$ approaches $f(a)$ when $x$ approaches $a$ (with values in $E$).

*Proof.* Left as a trivial exercise.

Another important proposition relating the notion of convergence of a sequence to continuity, is stated without proof.

**Proposition 2.13.** Let $(E, O_E)$ and $(F, O_F)$ be two topological spaces, and let $f : E \to F$ be a function.

1. If $f$ is continuous, then for every sequence $(x_n)_{n \in \mathbb{N}}$ in $E$, if $(x_n)$ converges to $a$, then $(f(x_n))$ converges to $f(a)$.

2. If $E$ is a metric space, and $(f(x_n))$ converges to $f(a)$ whenever $(x_n)$ converges to $a$, for every sequence $(x_n)_{n \in \mathbb{N}}$ in $E$, then $f$ is continuous.

A special case of Definition 19.13 will be used when $E$ and $F$ are (nontrivial) normed vector spaces with norms $\| \cdot \|_1$ and $\| \cdot \|_2$. Let $U$ be any nonempty open subset of $E$. We showed earlier that $E$ has no isolated points and that every set $\{v\}$ is closed, for every $v \in E$. Since $E$ is nontrivial, for every $v \in U$, there is a nontrivial open ball contained in $U$ (an open ball not reduced to its center). Then, for every $v \in U$, $A = U \setminus \{v\}$ is open and nonempty, and clearly, $v \in \overline{A}$. For any $v \in U$, if $f(x)$ approaches $b$ when $x$ approaches $v$ with values in $A = U \setminus \{v\}$, we say that $f(x)$ approaches $b$ when $x$ approaches $v$ with values $\neq v$ in $U$. This is denoted by

$$\lim_{x \to v, x \in U, x \neq v} f(x) = b.$$ 

**Remark:** Variations of the above case show up in the following case: $E = \mathbb{R}$, and $F$ is some arbitrary topological space. Let $A$ be some nonempty subset of $\mathbb{R}$, and let $f : A \to F$ be some function. For any $a \in A$, we say that $f$ is continuous on the right at $a$ if

$$\lim_{x \to a, x \in A \cap [a, +\infty]} f(x) = f(a).$$

We can define continuity on the left at $a$ in a similar fashion.

Let us consider another variation. Let $A$ be some nonempty subset of $\mathbb{R}$, and let $f : A \to F$ be some function. For any $a \in A$, we say that $f$ has a discontinuity of the first kind at $a$ if

$$\lim_{x \to a, x \in A \cap (-\infty, a]} f(x) = f(a_-)$$

We can define continuity on the left at $a$ in a similar fashion.
and
\[
\lim_{x \to a, x \in A \cap [a, +\infty[} f(x) = f(a_+)
\]
both exist, and either \( f(a-) \neq f(a) \), or \( f(a+) \neq f(a) \).

Note that it is possible that \( f(a-) = f(a+) \), but \( f \) is still discontinuous at \( a \) if this common value differs from \( f(a) \). Functions defined on a nonempty subset of \( \mathbb{R} \), and that are continuous, except for some points of discontinuity of the first kind, play an important role in analysis.

In a metric space, there is another important notion of continuity, namely uniform continuity.

**Definition 2.14.** Given two metric spaces, \((E, d_E)\) and \((F, d_F)\), a function, \(f: E \to F\), is **uniformly continuous** if for every \( \epsilon > 0 \), there is some \( \eta > 0 \), such that, for all \( a, b \in E \),

\[
\text{if } d_E(a, b) \leq \eta \text{ then } d_F(f(a), f(b)) \leq \epsilon.
\]

See Figures 19.22 and 19.23.

![Figure 2.22: The real valued function \( f(x) = \sqrt{x} \) is uniformly continuous over \((0, \infty)\). Fix \( \epsilon \). If the \( x \) values lie within the rose colored \( \eta \) strip, the \( y \) values always lie within the peach \( \epsilon \) strip.](image)

As we saw earlier, the metric on a metric space is uniformly continuous, and the norm on a normed metric space is uniformly continuous.

Before considering differentials, we need to look at the continuity of linear maps.
2.4 Continuous Linear and Multilinear Maps

If $E$ and $F$ are normed vector spaces, we first characterize when a linear map $f : E \to F$ is continuous.

**Proposition 2.14.** Given two normed vector spaces $E$ and $F$, for any linear map $f : E \to F$, the following conditions are equivalent:

(1) The function $f$ is continuous at 0.

(2) There is a constant $k \geq 0$ such that, 
$$
\|f(u)\| \leq k, \text{ for every } u \in E \text{ such that } \|u\| \leq 1.
$$

(3) There is a constant $k \geq 0$ such that, 
$$
\|f(u)\| \leq k\|u\|, \text{ for every } u \in E.
$$

(4) The function $f$ is continuous at every point of $E$.

**Proof.** Assume (1). Then for every $\epsilon > 0$, there is some $\eta > 0$ such that, for every $u \in E$, if $\|u\| \leq \eta$, then $\|f(u)\| \leq \epsilon$. Pick $\epsilon = 1$, so that there is some $\eta > 0$ such that, if $\|u\| \leq \eta$, then $\|f(u)\| \leq 1$. If $\|u\| \leq 1$, then $\|\eta u\| \leq \eta \|u\| \leq \eta$, and so, $\|f(\eta u)\| \leq 1$, that is, $\eta \|f(u)\| \leq 1$, which implies $\|f(u)\| \leq \eta^{-1}$. Thus, Condition (2) holds with $k = \eta^{-1}$.

Assume that (2) holds. If $u = 0$, then by linearity, $f(0) = 0$, and thus $\|f(0)\| \leq k\|0\|$ holds trivially for all $k \geq 0$. If $u \neq 0$, then $\|u\| > 0$, and since 
$$
\left\| \frac{u}{\|u\|} \right\| = 1,
$$

Figure 2.23: The real valued function $f(x) = 1/x$ is not uniformly continuous over $(0, \infty)$. Fix $\epsilon$. In order for the $y$ values to lie within the peach epsilon strip, the widths of the eta strips decrease as $x \to 0$. 
we have
\[ \left\| f \left( \frac{u}{\|u\|} \right) \right\| \leq k, \]
which implies that
\[ \|f(u)\| \leq k\|u\|. \]
Thus, Condition (3) holds.

If (3) holds, then for all \(u, v \in E\), we have
\[ \|f(v) - f(u)\| = \|f(v - u)\| \leq k\|v - u\|. \]
If \(k = 0\), then \(f\) is the zero function, and continuity is obvious. Otherwise, if \(k > 0\), for every \(\epsilon > 0\), if \(\|v - u\| \leq \frac{\epsilon}{k}\), then \(\|f(v - u)\| \leq \epsilon\), which shows continuity at every \(u \in E\). Finally, it is obvious that (4) implies (1). \(\square\)

Among other things, Proposition 19.14 shows that a linear map is continuous iff the image of the unit (closed) ball is bounded. Since a continuous linear map satisfies the condition \(\|f(u)\| \leq k\|u\|\) (for some \(k \geq 0\)), it is also uniformly continuous.

If \(E\) and \(F\) are normed vector spaces, the set of all continuous linear maps \(f : E \to F\) is denoted by \(\mathcal{L}(E; F)\).

Using Proposition 19.14, we can define a norm on \(\mathcal{L}(E; F)\) which makes it into a normed vector space. This definition has already been given in Chapter 7 (Vol. I) (Definition 7.7 (Vol. I)) but for the reader’s convenience, we repeat it here.

**Definition 2.15.** Given two normed vector spaces \(E\) and \(F\), for every continuous linear map \(f : E \to F\), we define the norm \(\|f\|\) of \(f\) as
\[ \|f\| = \inf \{k \geq 0 : \|f(x)\| \leq k\|x\|, \text{ for all } x \in E\} = \sup \{\|f(x)\| : \|x\| \leq 1\}. \]

From Definition 19.15, for every continuous linear map \(f \in \mathcal{L}(E; F)\), we have
\[ \|f(x)\| \leq \|f\|\|x\|, \]
for every \(x \in E\). It is easy to verify that \(\mathcal{L}(E; F)\) is a normed vector space under the norm of Definition 19.15. Furthermore, if \(E, F, G\), are normed vector spaces, and \(f : E \to F\) and \(g : F \to G\) are continuous linear maps, we have
\[ \|g \circ f\| \leq \|g\|\|f\|. \]

We can now show that when \(E = \mathbb{R}^n\) or \(E = \mathbb{C}^n\), with any of the norms \(\|\|_1\), \(\|\|_2\), or \(\|\|_\infty\), then every linear map \(f : E \to F\) is continuous.

**Proposition 2.15.** If \(E = \mathbb{R}^n\) or \(E = \mathbb{C}^n\), with any of the norms \(\|\|_1\), \(\|\|_2\), or \(\|\|_\infty\), and \(F\) is any normed vector space, then every linear map \(f : E \to F\) is continuous.
2.4. CONTINUOUS LINEAR AND MULTILINEAR MAPS

Proof. Let \((e_1, \ldots, e_n)\) be the standard basis of \(\mathbb{R}^n\) (a similar proof applies to \(\mathbb{C}^n\)). In view of Proposition 7.3 (Vol. I), it is enough to prove the proposition for the norm 

\[ \|x\|_\infty = \max\{|x_i| \mid 1 \leq i \leq n\}. \]

We have,

\[ \|f(v) - f(u)\| = \|f(v - u)\| = \left\| f\left( \sum_{1 \leq i \leq n} (v_i - u_i)e_i \right) \right\| = \left\| \sum_{1 \leq i \leq n} (v_i - u_i)f(e_i) \right\|, \]

and so,

\[ \|f(v) - f(u)\| \leq \left( \sum_{1 \leq i \leq n} \|f(e_i)\| \right) \max_{1 \leq i \leq n} |v_i - u_i| = \left( \sum_{1 \leq i \leq n} \|f(e_i)\| \right) \|v - u\|_\infty. \]

By the argument used in Proposition 19.14 to prove that (3) implies (4), \(f\) is continuous. \(\Box\)

Actually, we proved in Theorem 7.4 (Vol. I) that if \(E\) is a vector space of finite dimension, then any two norms are equivalent, so that they define the same topology. This fact together with Proposition 19.15 prove the following:

**Theorem 2.16.** If \(E\) is a vector space of finite dimension (over \(\mathbb{R}\) or \(\mathbb{C}\)), then all norms are equivalent (define the same topology). Furthermore, for any normed vector space \(F\), every linear map \(f: E \to F\) is continuous.

\[ \mathcal{Z} \] If \(E\) is a normed vector space of infinite dimension, a linear map \(f: E \to F\) may not be continuous. As an example, let \(E\) be the infinite vector space of all polynomials over \(\mathbb{R}\). Let 

\[ \|P(X)\| = \sup_{0 \leq x \leq 1} |P(x)|. \]

We leave as an exercise to show that this is indeed a norm. Let \(F = \mathbb{R}\), and let \(f: E \to F\) be the map defined such that, \(f(P(X)) = P(3)\). It is clear that \(f\) is linear. Consider the sequence of polynomials 

\[ P_n(X) = \left( \frac{X}{2} \right)^n. \]

It is clear that \(\|P_n\| = \left( \frac{1}{2} \right)^n\), and thus, the sequence \(P_n\) has the null polynomial as a limit. However, we have 

\[ f(P_n(X)) = P_n(3) = \left( \frac{3}{2} \right)^n, \]

and the sequence \(f(P_n(X))\) diverges to \(+\infty\). Consequently, in view of Proposition 19.13 (1), \(f\) is not continuous.
We now consider the continuity of multilinear maps. We treat explicitly bilinear maps, the general case being a straightforward extension.

**Proposition 2.17.** Given normed vector spaces $E$, $F$ and $G$, for any bilinear map $f: E \times E \to G$, the following conditions are equivalent:

1) The function $f$ is continuous at $(0,0)$.

2) There is a constant $k \geq 0$ such that,
   $$\|f(u,v)\| \leq k,$$
   for all $u, v \in E$ such that $\|u\|, \|v\| \leq 1$.

3) There is a constant $k \geq 0$ such that,
   $$\|f(u,v)\| \leq k\|u\|\|v\|,$$
   for all $u, v \in E$.

4) The function $f$ is continuous at every point of $E \times F$.

**Proof.** It is similar to that of Proposition 19.14, with a small subtlety in proving that (3) implies (4), namely that two different $\eta$’s that are not independent are needed.

In contrast to continuous linear maps, which must be uniformly continuous, nonzero continuous bilinear maps are not uniformly continuous. Let $f: E \times F \to G$ be a continuous bilinear map such that $f(a,b) \neq 0$ for some $a \in E$ and some $b \in F$. Consider the sequences $(u_n)$ and $(v_n)$ (with $n \geq 1$) given by

$$u_n = (x_n, y_n) = (na, nb)$$

$$v_n = (x'_n, y'_n) = \left(\left(n + \frac{1}{n}\right)a, \left(n + \frac{1}{n}\right)b\right).$$

Obviously

$$\|v_n - u_n\| \leq \frac{1}{n}(\|a\| + \|b\|),$$

so $\lim_{n \to \infty} \|v_n - u_n\| = 0$. On the other hand

$$f(x'_n, y'_n) - f(x_n, y_n) = \left(2 + \frac{1}{n^2}\right)f(a, b),$$

and thus $\lim_{n \to \infty} \|f(x'_n, y'_n) - f(x_n, y_n)\| = 2\|f(a, b)\| \neq 0$, which shows that $f$ is not uniformly continuous, because if this was the case, this limit would be zero.

If $E$, $F$, and $G$, are normed vector spaces, we denote the set of all continuous bilinear maps $f: E \times F \to G$ by $\mathcal{L}_2(E,F;G)$. Using Proposition 19.17, we can define a norm on $\mathcal{L}_2(E,F;G)$ which makes it into a normed vector space.
Definition 2.16. Given normed vector spaces $E$, $F$, and $G$, for every continuous bilinear map $f: E \times F \to G$, we define the norm $\|f\|$ of $f$ as

$$
\|f\| = \inf \{ k \geq 0 \mid \|f(x, y)\| \leq k\|x\|\|y\|, \text{ for all } x, y \in E \}
$$

$$
= \sup \{ \|f(x, y)\| \mid \|x\|, \|y\| \leq 1 \}.
$$

From Definition 19.15, for every continuous bilinear map $f \in L_2(E, F; G)$, we have

$$
\|f(x, y)\| \leq \|f\|\|x\|\|y\|,
$$

for all $x, y \in E$. It is easy to verify that $L_2(E, F; G)$ is a normed vector space under the norm of Definition 19.16.

Given a bilinear map $f: E \times F \to G$, for every $u \in E$, we obtain a linear map denoted $fu: F \to G$, defined such that, $fu(v) = f(u, v)$. Furthermore, since

$$
\|f(x, y)\| \leq \|f\|\|x\|\|y\|,
$$

it is clear that $fu$ is continuous. We can then consider the map $\varphi: E \to L(F; G)$, defined such that, $\varphi(u) = fu$, for any $u \in E$, or equivalently, such that,

$$
\varphi(u)(v) = f(u, v).
$$

Actually, it is easy to show that $\varphi$ is linear and continuous, and that $\|\varphi\| = \|f\|$. Thus, $f \mapsto \varphi$ defines a map from $L_2(E, F; G)$ to $L(E; L(F; G))$. We can also go back from $L(E; L(F; G))$ to $L_2(E, F; G)$. We summarize all this in the following proposition.

Proposition 2.18. Let $E, F, G$ be three normed vector spaces. The map $f \mapsto \varphi$, from $L_2(E, F; G)$ to $L(E; L(F; G))$, defined such that, for every $f \in L_2(E, F; G)$,

$$
\varphi(u)(v) = f(u, v),
$$

is an isomorphism of vector spaces, and furthermore, $\|\varphi\| = \|f\|$.

As a corollary of Proposition 19.18, we get the following proposition which will be useful when we define second-order derivatives.

Proposition 2.19. Let $E, F$ be normed vector spaces. The map $\text{app}$ from $L(E; F) \times E$ to $F$, defined such that, for every $f \in L(E; F)$, for every $u \in E$,

$$
\text{app}(f, u) = f(u),
$$

is a continuous bilinear map.
Remark: If $E$ and $F$ are nontrivial, it can be shown that $\|\text{app}\| = 1$. It can also be shown that composition

$$\circ : \mathcal{L}(E; F) \times \mathcal{L}(F; G) \to \mathcal{L}(E; G),$$

is bilinear and continuous.

The above propositions and definition generalize to arbitrary $n$-multilinear maps, with $n \geq 2$. Proposition 19.17 extends in the obvious way to any $n$-multilinear map $f : E_1 \times \cdots \times E_n \to F$, but condition (3) becomes:

There is a constant $k \geq 0$ such that,

$$\|f(u_1, \ldots, u_n)\| \leq k\|u_1\| \cdots \|u_n\|, \text{ for all } u_1 \in E_1, \ldots, u_n \in E_n.$$

Definition 19.16 also extends easily to

$$\|f\| = \inf\{k \geq 0 \mid \|f(x_1, \ldots, x_n)\| \leq k\|x_1\| \cdots \|x_n\|, \text{ for all } x_i \in E_i, 1 \leq i \leq n\} = \sup\{\|f(x_1, \ldots, x_n)\| \mid \|x_i\|, \ldots, \|x_n\| \leq 1\}.$$

Proposition 19.18 is also easily extended, and we get an isomorphism between continuous $n$-multilinear maps in $\mathcal{L}_n(E_1, \ldots, E_n; F)$, and continuous linear maps in

$$\mathcal{L}(E_1; \mathcal{L}(E_2; \cdots; \mathcal{L}(E_n; F))).$$

An obvious extension of Proposition 19.19 also holds.

Complete metric spaces and complete normed vector spaces are important tools in analysis and optimization theory, so we include some sections covering the basics.

## 2.5 Complete Metric Spaces and Banach Spaces

**Definition 2.17.** Given a metric space, $(E, d)$, a sequence, $(x_n)_{n \in \mathbb{N}}$, in $E$ is a Cauchy sequence if the following condition holds: for every $\epsilon > 0$, there is some $p \geq 0$, such that, for all $m, n \geq p$, then $d(x_m, x_n) \leq \epsilon$.

If every Cauchy sequence in $(E, d)$ converges we say that $(E, d)$ is a complete metric space. A normed vector space $(E, \|\|)$ over $\mathbb{R}$ (or $\mathbb{C}$) which is a complete metric space for the distance $d(u, v) = \|v - u\|$, is called a Banach space.

The standard example of a complete metric space is the set $\mathbb{R}$ of real numbers. As a matter of fact, the set $\mathbb{R}$ can be defined as the “completion” of the set $\mathbb{Q}$ of rationals. The spaces $\mathbb{R}^n$ and $\mathbb{C}^n$ under their standard topology are complete metric spaces.

It can be shown that every normed vector space of finite dimension is a Banach space (is complete). It can also be shown that if $E$ and $F$ are normed vector spaces, and $F$ is a
Banach space, then $L(E;F)$ is a Banach space. If $E, F$ and $G$ are normed vector spaces, and $G$ is a Banach space, then $L_2(E, F; G)$ is a Banach space.

An arbitrary metric space $(E, d)$ is not necessarily complete, but there is a construction of a metric space $(\hat{E}, \hat{d})$ such that $\hat{E}$ is complete, and there is a continuous (injective) distance-preserving map $\varphi: E \to \hat{E}$ such that $\varphi(E)$ is dense in $\hat{E}$. This is a generalization of the construction of the set $\mathbb{R}$ of real numbers from the set $\mathbb{Q}$ of rational numbers in terms of Cauchy sequences. This construction can be immediately adapted to a normed vector space $(E, \|\|)$ to embed $(E, \|\|)$ into a complete normed vector space $(\hat{E}, \|\|_{\hat{E}})$ (a Banach space). This construction is used heavily in integration theory, where $E$ is a set of functions.

## 2.6 Completion of a Metric Space

In order to prove a kind of uniqueness result for the completion $(\hat{E}, \hat{d})$ of a metric space $(E, d)$, we need the following result about extending a uniformly continuous function.

Recall that $E_0$ is dense in $E$ iff $\overline{E_0} = E$. Since $E$ is a metric space, by Proposition 19.11, this means that for every $x \in E$, there is some sequence $(x_n)$ converging to $x$, with $x_n \in E_0$.

**Theorem 2.20.** Let $E$ and $F$ be two metric spaces, let $E_0$ be a dense subspace of $E$, and let $f_0: E_0 \to F$ be a continuous function. If $f_0$ is uniformly continuous and if $F$ is complete, then there is a unique uniformly continuous function $f: E \to F$ extending $f_0$.

**Proof.** We follow Schwartz’s proof; see Schwartz [90] (Chapter XI, Section 3, Theorem 1).

**Step 1.** We begin by constructing a function $f: E \to F$ extending $f_0$. Since $E_0$ is dense in $E$, for every $x \in E$, there is some sequence $(x_n)$ converging to $x$, with $x_n \in E_0$. Then the sequence $(x_n)$ is a Cauchy sequence in $E$. We claim that $(f_0(x_n))$ is a Cauchy sequence in $F$.

**Proof of the claim.** For every $\epsilon > 0$, since $f_0$ is uniformly continuous, there is some $\eta > 0$ such that for all $(y, z) \in E_0$, if $d(y, z) \leq \eta$, then $d(f_0(y), f_0(z)) \leq \epsilon$. Since $(x_n)$ is a Cauchy sequence with $x_n \in E_0$, there is some integer $p > 0$ such that if $m, n \geq p$, then $d(x_m, x_n) \leq \eta$, thus $d(f_0(x_m), f_0(x_n)) \leq \epsilon$, which proves that $(f_0(x_n))$ is a Cauchy sequence in $F$. \qed

Since $F$ is complete and $(f_0(x_n))$ is a Cauchy sequence in $F$, the sequence $(f_0(x_n))$ converges to some element of $F$; denote this element by $f(x)$.

**Step 2.** Let us now show that $f(x)$ does not depend on the sequence $(x_n)$ converging to $x$. Suppose that $(x'_n)$ and $(x''_n)$ are two sequences of elements in $E_0$ converging to $x$. Then the mixed sequence

$$x'_0, x'_0, x'_1, x''_1, \ldots, x'_n, x''_n, \ldots,$$

also converges to $x$. It follows that the sequence

$$f_0(x'_0), f_0(x'_0), f_0(x'_1), f_0(x'_1), \ldots, f_0(x'_n), f_0(x''_n), \ldots,$$

is a metric space ($E, d$) such that $E$ is complete, and there is a continuous (injective) distance-preserving map $\varphi: E \to \hat{E}$ such that $\varphi(E)$ is dense in $\hat{E}$. This is a generalization of the construction of the set $\mathbb{R}$ of real numbers from the set $\mathbb{Q}$ of rational numbers in terms of Cauchy sequences. This construction can be immediately adapted to a normed vector space $(E, \|\|)$ to embed $(E, \|\|)$ into a complete normed vector space $(\hat{E}, \|\|_{\hat{E}})$ (a Banach space). This construction is used heavily in integration theory, where $E$ is a set of functions.
is a Cauchy sequence in $F$, and since $F$ is complete, it converges to some element of $F$, which implies that the sequences $(f_0(x'_n))$ and $(f_0(x''_n))$ converge to the same limit.

As a summary, we have defined a function $f : E \to F$ by

$$f(x) = \lim_{n \to \infty} f_0(x_n).$$

for any sequence $(x_n)$ converging to $x$, with $x_n \in E_0$.

**Step 3.** The function $f$ extends $f_0$. Since every element $x \in E_0$ is the limit of the constant sequence $(x_n)$ with $x_n = x$ for all $n \geq 0$, by definition $f(x)$ is the limit of the sequence $(f_0(x_n))$, which is the constant sequence with value $f_0(x)$, so $f(x) = f_0(x)$; that is, $f$ extends $f_0$.

**Step 4.** We now prove that $f$ is uniformly continuous. Since $f_0$ is uniformly continuous, for every $\epsilon > 0$, there is some $\eta > 0$ such that if $a, b \in E_0$ and $d(a, b) \leq \eta$, then $d(f_0(a), f_0(b)) \leq \epsilon$. Consider any two points $x, y \in E$ such that $d(x, y) \leq \eta/2$. We claim that $d(f(x), f(y)) \leq \epsilon$, which shows that $f$ is uniformly continuous.

Let $(x_n)$ be a sequence of points in $E_0$ converging to $x$, and let $(y_n)$ be a sequence of points in $E_0$ converging to $y$. By the triangle inequality,

$$d(x_n, y_n) \leq d(x_n, x) + d(x, y) + d(y, y_n) = d(x, y) + d(x_n, x) + d(y_n, y),$$

and since $(x_n)$ converges to $x$ and $(y_n)$ converges to $y$, there is some integer $p > 0$ such that for all $n \geq p$, we have $d(x_n, x) \leq \eta/4$ and $d(y_n, y) \leq \eta/4$, and thus

$$d(x_n, y_n) \leq d(x, y) + \frac{\eta}{2}.$$ 

Since we assumed that $d(x, y) \leq \eta/2$, we get $d(x_n, y_n) \leq \eta$ for all $n \geq p$, and by uniform continuity of $f_0$, we get

$$d(f_0(x_n), f_0(y_n)) \leq \epsilon$$

for all $n \geq p$. Since the distance function on $F$ is also continuous, and since $(f_0(x_n))$ converges to $f(x)$ and $(f_0(y_n))$ converges to $f(y)$, we deduce that the sequence $(d(f_0(x_n), f_0(y_n)))$ converges to $d(f(x), f(y))$. This implies that $d(f(x), f(y)) \leq \epsilon$, as desired.

**Step 5.** It remains to prove that $f$ is unique. Since $E_0$ is dense in $E$, for every $x \in E$, there is some sequence $(x_n)$ converging to $x$, with $x_n \in E_0$. Since $f$ extends $f_0$ and since $f$ is continuous, we get

$$f(x) = \lim_{n \to \infty} f_0(x_n),$$

which only depends on $f_0$ and $x$, and shows that $f$ is unique. \qed

**Remark:** It can be shown that the theorem no longer holds if we either omit the hypothesis that $F$ is complete or omit that $f_0$ is uniformly continuous.
For example, if \( E_0 \neq E \) and if we let \( F = E_0 \) and \( f_0 \) be the identity function, it is easy to see that \( f_0 \) cannot be extended to a continuous function from \( E \) to \( E_0 \) (for any \( x \in E - E_0 \), any continuous extension \( f \) of \( f_0 \) would satisfy \( f(x) = x \), which is absurd since \( x \notin E_0 \)).

If \( f_0 \) is continuous but not uniformly continuous, a counter-example can be given by using \( E = \mathbb{R} = \mathbb{R} \cup \{\infty\} \) made into a metric space, \( E_0 = \mathbb{R} \), \( F = \mathbb{R} \), and \( f_0 \) the identity function; for details, see Schwartz [90] (Chapter XI, Section 3, page 134).

**Definition 2.18.** If \((E,d_E)\) and \((F,d_F)\) are two metric spaces, then a function \( f: E \to F \) is distance-preserving, or an isometry, if
\[
d_F(f(x), f(y)) = d_E(x, y), \quad \text{for all for all } x, y \in E.
\]

Observe that an isometry must be injective, because if \( f(x) = f(y) \), then \( d_F(f(x), f(y)) = 0 \), and since \( d_F(f(x), f(y)) = d_E(x, y) \), we get \( d_E(x, y) = 0 \), but \( d_E(x, y) = 0 \) implies that \( x = y \). Also, an isometry is uniformly continuous (since we can pick \( \eta = \epsilon \) to satisfy the condition of uniform continuity). However, an isometry is not necessarily surjective.

We now give a construction of the completion of a metric space. This construction is just a generalization of the classical construction of \( \mathbb{R} \) from \( \mathbb{Q} \) using Cauchy sequences.

**Theorem 2.21.** Let \( (E,d) \) be any metric space. There is a complete metric space \( (\hat{E}, \hat{d}) \) called a completion of \( (E,d) \), and a distance-preserving (uniformly continuous) map \( \varphi: E \to \hat{E} \) such that \( \varphi(E) \) is dense in \( \hat{E} \), and the following extension property holds: for every complete metric space \( F \) and for every uniformly continuous function \( f: E \to F \), there is a unique uniformly continuous function \( \hat{f}: \hat{E} \to F \) such that
\[
f = \hat{f} \circ \varphi,
\]
as illustrated in the following diagram.

\[
E \xrightarrow{\varphi} \hat{E} \\
\downarrow f \downarrow \hat{f} \\
F.
\]

As a consequence, for any two completions \( (\hat{E}_1, \hat{d}_1) \) and \( (\hat{E}_2, \hat{d}_2) \) of \( (E,d) \), there is a unique bijective isometry between \( (\hat{E}_1, \hat{d}_1) \) and \( (\hat{E}_2, \hat{d}_2) \).

**Proof.** Consider the set \( \mathcal{E} \) of all Cauchy sequences \( (x_n) \) in \( E \), and define the relation \( \sim \) on \( \mathcal{E} \) as follows:
\[
(x_n) \sim (y_n) \iff \lim_{n \to \infty} d(x_n, y_n) = 0.
\]

It is easy to check that \( \sim \) is an equivalence relation on \( \mathcal{E} \), and let \( \hat{E} = \mathcal{E} / \sim \) be the quotient set, that is, the set of equivalence classes modulo \( \sim \). Our goal is to show that we can endow
\( \hat{E} \) with a distance that makes it into a complete metric space satisfying the conditions of the theorem. We proceed in several steps.

**Step 1.** First, let us construct the function \( \varphi : E \to \hat{E} \). For every \( a \in E \), we have the constant sequence \( (a_n) \) such that \( a_n = a \) for all \( n \geq 0 \), which is obviously a Cauchy sequence. Let \( \varphi(a) \in \hat{E} \) be the equivalence class \([ (a_n) ]\) of the constant sequence \( (a_n) \) with \( a_n = a \) for all \( n \). By definition of \( \sim \), the equivalence class \( \varphi(a) \) is also the equivalence class of all sequences converging to \( a \). The map \( a \mapsto \varphi(a) \) is injective because a metric space is Hausdorff, so if \( a \neq b \), then a sequence converging to \( a \) does not converge to \( b \). After having defined a distance on \( \hat{E} \), we will check that \( \varphi \) is an isometry.

**Step 2.** Let us now define a distance on \( \hat{E} \). Let \( \alpha = [(a_n)] \) and \( \beta = [(b_n)] \) be two equivalence classes of Cauchy sequences in \( E \). The triangle inequality implies that

\[
d(a_m, b_m) \leq d(a_m, a_n) + d(a_n, b_n) + d(b_n, b_m) = d(a_n, b_n) + d(a_m, a_n) + d(b_m, b_n)
\]

and

\[
d(a_n, b_n) \leq d(a_n, a_m) + d(a_m, b_m) + d(b_m, b_n) = d(a_m, b_m) + d(a_m, a_n) + d(b_m, b_n),
\]

which implies that

\[
|d(a_m, b_m) - d(a_n, b_n)| \leq d(a_m, a_n) + d(b_m, b_n).
\]

Since \( (a_n) \) and \( (b_n) \) are Cauchy sequences, it follows that \( (d(a_n, b_n)) \) is a Cauchy sequence of nonnegative reals. Since \( \mathbb{R} \) is complete, the sequence \( (d(a_n, b_n)) \) has a limit, which we denote by \( \hat{d}(\alpha, \beta) \); that is, we set

\[
\hat{d}(\alpha, \beta) = \lim_{n \to \infty} d(a_n, b_n), \quad \alpha = [(a_n)], \; \beta = [(b_n)].
\]

**Step 3.** Let us check that \( \hat{d}(\alpha, \beta) \) does not depend on the Cauchy sequences \( (a_n) \) and \( (b_n) \) chosen in the equivalence classes \( \alpha \) and \( \beta \).

If \( (a_n) \sim (a'_n) \) and \( (b_n) \sim (b'_n) \), then \( \lim_{n \to \infty} d(a_n, a'_n) = 0 \) and \( \lim_{n \to \infty} d(b_n, b'_n) = 0 \), and since

\[
d(a'_n, b'_n) \leq d(a'_n, a_n) + d(a_n, b_n) + d(b_n, b'_n) = d(a_n, b_n) + d(a_n, a'_n) + d(b_n, b'_n)
\]

and

\[
d(a_n, b_n) \leq d(a_n, a'_n) + d(a'_n, b'_n) + d(b'_n, b_n) = d(a'_n, b'_n) + d(a_n, a'_n) + d(b_n, b'_n)
\]

we have

\[
|d(a_n, b_n) - d(a'_n, b'_n)| \leq d(a_n, a'_n) + d(b_n, b'_n),
\]

so we have \( \lim_{n \to \infty} d(a'_n, b'_n) = \lim_{n \to \infty} d(a_n, b_n) = \hat{d}(\alpha, \beta) \). Therefore, \( \hat{d}(\alpha, \beta) \) is indeed well defined.
Step 4. Let us check that \( \varphi \) is indeed an isometry.

Given any two elements \( \varphi(a) \) and \( \varphi(b) \) in \( \widehat{E} \), since they are the equivalence classes of the constant sequences \( (a_n) \) and \( (b_n) \) such that \( a_n = a \) and \( b_n = b \) for all \( n \), the constant sequence \( (d(a_n, b_n)) \) with \( d(a_n, b_n) = d(a, b) \) for all \( n \) converges to \( d(a, b) \), so by definition \( \widehat{d}(\varphi(a), \varphi(b)) = \lim_{n \to \infty} d(a_n, b_n) = d(a, b) \), which shows that \( \varphi \) is an isometry.

Step 5. Let us verify that \( \widehat{d} \) is a metric on \( \widehat{E} \). By definition it is obvious that \( \widehat{d}(\alpha, \beta) = \widehat{d}(\beta, \alpha) \). If \( \alpha \) and \( \beta \) are two distinct equivalence classes, then for any Cauchy sequence \( (a_n) \) in the equivalence class \( \alpha \) and for any Cauchy sequence \( (b_n) \) in the equivalence class \( \beta \), the sequences \( (a_n) \) and \( (b_n) \) are inequivalent, which means that \( \lim_{n \to \infty} d(a_n, b_n) \neq 0 \), that is, \( \widehat{d}(\alpha, \beta) \neq 0 \). Obviously, \( \widehat{d}(\alpha, \alpha) = 0 \).

For any equivalence classes \( \alpha = [(a_n)], \beta = [(b_n)], \) and \( \gamma = [(c_n)] \), we have the triangle inequality

\[
\widehat{d}(a_n, c_n) \leq \widehat{d}(a_n, b_n) + \widehat{d}(b_n, c_n),
\]

so by continuity of the distance function, by passing to the limit, we obtain

\[
\widehat{d}(\alpha, \gamma) \leq \widehat{d}(\alpha, \beta) + \widehat{d}(\beta, \gamma),
\]

which is the triangle inequality for \( \widehat{d} \). Therefore, \( \widehat{d} \) is a distance on \( \widehat{E} \).

Step 6. Let us prove that \( \varphi(E) \) is dense in \( \widehat{E} \). For any \( \alpha = [(a_n)] \), let \( (x_n) \) be the constant sequence such that \( x_k = a_n \) for all \( k \geq 0 \), so that \( \varphi(a_n) = [(x_n)] \). Then we have

\[
\widehat{d}(\alpha, \varphi(a_n)) = \lim_{m \to \infty} d(a_m, a_n) \leq \sup_{p,q \geq n} d(a_p, a_q).
\]

Since \( (a_n) \) is a Cauchy sequence, \( \sup_{p,q \geq n} d(a_p, a_q) \) tends to 0 as \( n \) goes to infinity, so

\[
\lim_{n \to \infty} \widehat{d}(\alpha, \varphi(a_n)) = 0,
\]

which means that the sequence \( \varphi(a_n) \) converge to \( \alpha \), and \( \varphi(E) \) is indeed dense in \( \widehat{E} \).

Step 7. Finally, let us prove that the metric space \( \widehat{E} \) is complete.

Let \( (\alpha_n) \) be a Cauchy sequence in \( \widehat{E} \). Since \( \varphi(E) \) is dense in \( \widehat{E} \), for every \( n > 0 \), there some \( a_n \in E \) such that

\[
\widehat{d}(\alpha_n, \varphi(a_n)) \leq \frac{1}{n}.
\]

Since

\[
\widehat{d}(\varphi(a_m), \varphi(a_n)) \leq \widehat{d}(\varphi(a_m), \alpha_m) + \widehat{d}(\alpha_m, \alpha_n) + \widehat{d}(\alpha_n, \varphi(a_n)) \leq \widehat{d}(\alpha_m, \alpha_n) + \frac{1}{m} + \frac{1}{n},
\]

and since \( (\alpha_m) \) is a Cauchy sequence, so is \( (\varphi(a_n)) \), and as \( \varphi \) is an isometry, the sequence \( (a_n) \) is a Cauchy sequence in \( E \). Let \( \alpha \in \widehat{E} \) be the equivalence class of \( (a_n) \). Since

\[
\widehat{d}(\alpha, \varphi(a_n)) = \lim_{m \to \infty} \widehat{d}(a_m, a_n)
\]
and $(a_n)$ is a Cauchy sequence, we deduce that the sequence $(\varphi(a_n))$ converges to $\alpha$, and since $d(\alpha_n, \varphi(a_n)) \leq 1/n$ for all $n > 0$, the sequence $(\alpha_n)$ also converges to $\alpha$.

**Step 8.** Let us prove the extension property. Let $F$ be any complete metric space and let $f: E \to F$ be any uniformly continuous function. The function $\varphi: E \to \hat{E}$ is an isometry and a bijection between $E$ and its image $\varphi(E)$, so its inverse $\varphi^{-1}: \varphi(E) \to E$ is also an isometry, and thus is uniformly continuous. If we let $g = f \circ \varphi^{-1}$, then $g: \varphi(E) \to F$ is a uniformly continuous function, and $\varphi(E)$ is dense in $\hat{E}$, so by Theorem 19.20 there is a unique uniformly continuous function $\hat{f}: \hat{E} \to F$ extending $g = f \circ \varphi^{-1}$; see the diagram below:

This means that $\hat{f}|\varphi(E) = f \circ \varphi^{-1}$,

which implies that $(\hat{f}|\varphi(E)) \circ \varphi = f$,

that is, $f = \hat{f} \circ \varphi$, as illustrated in the diagram below:

If $h: \hat{E} \to F$ is any other uniformly continuous function such that $f = h \circ \varphi$, then $g = f \circ \varphi^{-1} = h|\varphi(E)$, so $h$ is a uniformly continuous function extending $g$, and by Theorem 19.20, we have have $h = \hat{f}$, so $\hat{f}$ is indeed unique.

**Step 9.** Uniqueness of the completion $(\hat{E}, \hat{d})$ up to a bijective isometry.

Let $(\hat{E}_1, \hat{d}_1)$ and $(\hat{E}_2, \hat{d}_2)$ be any two completions of $(E, d)$. Then we have two uniformly continuous isometries $\varphi_1: E \to \hat{E}_1$ and $\varphi_2: E \to \hat{E}_2$, so by the unique extension property, there exist unique uniformly continuous maps $\hat{\varphi}_2: \hat{E}_1 \to \hat{E}_2$ and $\hat{\varphi}_1: \hat{E}_2 \to \hat{E}_1$ such that the following diagrams commute:

$$
\begin{align*}
E & \xrightarrow{\varphi_1} \hat{E}_1 & E & \xrightarrow{\varphi_2} \hat{E}_2 \\
\varphi_2 & \downarrow \hat{\varphi}_2 & \varphi_1 & \downarrow \hat{\varphi}_1 \\
\hat{E}_2 & & \hat{E}_1.
\end{align*}
$$
2.6. COMPLETION OF A METRIC SPACE

Consequently we have the following commutative diagrams:

\[
\begin{array}{ccc}
E & \xrightarrow{\varphi_1} & \hat{E}_1 \\
\downarrow & & \downarrow \\
\varphi_2 & & \varphi_2 \\
\hat{E}_2 & & \hat{E}_2 \\
\end{array}
\quad
\begin{array}{ccc}
E & \xrightarrow{\varphi_2} & \hat{E}_2 \\
\downarrow & & \downarrow \\
\varphi_1 & & \varphi_1 \\
\hat{E}_1 & & \hat{E}_1 \\
\end{array}
\]

However, \(\text{id}_{\hat{E}_1}\) and \(\text{id}_{\hat{E}_2}\) are uniformly continuous functions making the following diagrams commute

\[
\begin{array}{ccc}
E & \xrightarrow{\varphi_1} & \hat{E}_1 \\
\downarrow & & \downarrow \text{id}_{\hat{E}_1} \\
\hat{E}_1 & & \hat{E}_1 \\
\end{array}
\quad
\begin{array}{ccc}
E & \xrightarrow{\varphi_2} & \hat{E}_2 \\
\downarrow & & \downarrow \text{id}_{\hat{E}_2} \\
\hat{E}_2 & & \hat{E}_2 \\
\end{array}
\]

so by the uniqueness of extensions we must have

\[
\varphi_1 \circ \varphi_2 = \text{id}_{\hat{E}_1} \quad \text{and} \quad \varphi_2 \circ \varphi_1 = \text{id}_{\hat{E}_2}.
\]

This proves that \(\hat{\varphi}_1\) and \(\hat{\varphi}_2\) are mutual inverses. Now, since \(\varphi_2 = \hat{\varphi}_2 \circ \varphi_1\), we have

\[
\varphi_2 | \varphi_1(E) = \varphi_2 \circ \varphi_1^{-1},
\]

and since \(\varphi_1^{-1}\) and \(\varphi_2\) are isometries, so is \(\hat{\varphi}_2 | \varphi_1(E)\). But we saw earlier that \(\hat{\varphi}_2\) is the uniform continuous extension of \(\varphi_2 | \varphi_1(E)\) and \(\varphi_1(E)\) is dense in \(\hat{E}_1\), so for any two elements \(\alpha, \beta \in \hat{E}_1\), if \((a_n)\) and \((b_n)\) are sequences in \(\varphi_1(E)\) converging to \(\alpha\) and \(\beta\), we have

\[
\hat{d}_2(\hat{\varphi}_2 | \varphi_1(E))(a_n), ((\hat{\varphi}_2 | \varphi_1(E))(b_n)) = \hat{d}_1(a_n, b_n),
\]

and by passing to the limit we get

\[
\hat{d}_2(\hat{\varphi}_2(\alpha), \hat{\varphi}_2(\beta)) = \hat{d}_1(\alpha, \beta),
\]

which shows that \(\hat{\varphi}_2\) is an isometry (similarly, \(\hat{\varphi}_1\) is an isometry). \(\square\)

Remarks:

1. Except for Step 8 and Step 9, the proof of Theorem 19.21 is the proof given in Schwartz [90] (Chapter XI, Section 4, Theorem 1), and Kormogorov and Fomin [61] (Chapter 2, Section 7, Theorem 4).

2. The construction of \(\hat{E}\) relies on the completeness of \(\mathbb{R}\), and so it cannot be used to construct \(\mathbb{R}\) from \(\mathbb{Q}\). However, this construction can be modified to yield a construction of \(\mathbb{R}\) from \(\mathbb{Q}\).

We show in Section 19.7 that Theorem 19.21 yields a construction of the completion of a normed vector space.
2.7 Completion of a Normed Vector Space

An easy corollary of Theorem 19.21 and Theorem 19.20 is that every normed vector space can be embedded in a complete normed vector space, that is, a Banach space.

**Theorem 2.22.** If $(E, \|\|)$ is a normed vector space, then its completion $(\hat{E}, \hat{d})$ as a metric space (where $E$ is given the metric $d(x, y) = \|x - y\|$) can be given a unique vector space structure extending the vector space structure on $E$, and a norm $\|\|_{\hat{E}}$, so that $(\hat{E}, \|\|_{\hat{E}})$ is a Banach space, and the metric $\hat{d}$ is associated with the norm $\|\|_{\hat{E}}$. Furthermore, the isometry $\varphi: E \to \hat{E}$ is a linear isometry.

**Proof.** The addition operation $+: E \times E \to E$ is uniformly continuous because

$$\|(u' + v') - (u'' + v'')\| \leq \|u' - u''\| + \|v' - v''\|.$$ 

It is not hard to show that $\hat{E} \times \hat{E}$ is a complete metric space and that $E \times E$ is dense in $\hat{E} \times \hat{E}$. Then, by Theorem 19.20, the uniformly continuous function $+$ has a unique continuous extension $+: \hat{E} \times \hat{E} \to \hat{E}$.

The map $\cdot: \mathbb{R} \times E \to E$ is not uniformly continuous, but for any fixed $\lambda \in \mathbb{R}$, the map $L_\lambda: E \to E$ given by $L_\lambda(u) = \lambda \cdot u$ is uniformly continuous, so by Theorem 19.20 the function $L_\lambda$ has a unique continuous extension $L_\lambda: \hat{E} \to \hat{E}$, which we use to define the scalar multiplication $\cdot: \mathbb{R} \times \hat{E} \to \hat{E}$. It is easily checked that with the above addition and scalar multiplication, $\hat{E}$ is a vector space.

Since the norm $\|\|$ on $E$ is uniformly continuous, it has a unique continuous extension $\|\|_{\hat{E}}: \hat{E} \to \mathbb{R}_+$. The identities $\|u + v\| \leq \|u\| + \|v\|$ and $\|\lambda u\| \leq |\lambda| \|u\|$ extend to $\hat{E}$ by continuity. The equation

$$d(u, v) = \|u - v\|$$

also extends to $\hat{E}$ by continuity and yields

$$\hat{d}(\alpha, \beta) = \|\alpha - \beta\|_{\hat{E}},$$

which shows that $\|\|_{\hat{E}}$ is indeed a norm, and that the metric $\hat{d}$ is associated to it. Finally, it is easy to verify that the map $\varphi$ is linear. The uniqueness of the structure of normed vector space follows from the uniqueness of continuous extensions in Theorem 19.20.

Theorem 19.22 and Theorem 19.20 will be used to show that every Hermitian space can be embedded in a Hilbert space.

We refer the readers to the references cited at the end of this chapter for a discussion of the concepts of compactness and connectedness. They are important, but of less immediate concern.
2.8 The Contraction Mapping Theorem

If \((E, d)\) is a nonempty complete metric space, every map, \(f: E \to E\), for which there is some \(k\) such that \(0 \leq k < 1\) and

\[
d(f(x), f(y)) \leq kd(x, y) \quad \text{for all } x, y \in E
\]

has the very important property that it has a unique fixed point, that is, there is a unique, \(a \in E\), such that \(f(a) = a\).

**Definition 2.19.** Let \((E, d)\) be a metric space. A map \(f: E \to E\) is a contraction (or a contraction mapping) if there is some real number \(k\) such that \(0 \leq k < 1\) and

\[
d(f(u), f(v)) \leq kd(u, v) \quad \text{for all } u, v \in E.
\]

The number \(k\) is often called a Lipschitz constant.

Furthermore, the fixed point of a contraction mapping can be computed as the limit of a fast converging sequence.

The fixed point property of contraction mappings is used to show some important theorems of analysis, such as the implicit function theorem and the existence of solutions to certain differential equations. It can also be used to show the existence of fractal sets defined in terms of iterated function systems. Since the proof is quite simple, we prove the fixed point property of contraction mappings. First, observe that a contraction mapping is (uniformly) continuous.

**Theorem 2.23.** (Contraction Mapping Theorem) If \((E, d)\) is a nonempty complete metric space, every contraction mapping, \(f: E \to E\), has a unique fixed point. Furthermore, for every \(x_0 \in E\), if we define the sequence \((x_n)_{n \geq 0}\) such that \(x_{n+1} = f(x_n)\) for all \(n \geq 0\), then \((x_n)_{n \geq 0}\) converges to the unique fixed point of \(f\).

**Proof.** First we prove that \(f\) has at most one fixed point. Indeed, if \(f(a) = a\) and \(f(b) = b\), since

\[
d(a, b) = d(f(a), f(b)) \leq kd(a, b)
\]

and \(0 \leq k < 1\), we must have \(d(a, b) = 0\), that is, \(a = b\).

Next we prove that \((x_n)\) is a Cauchy sequence. Observe that

\[
d(x_2, x_1) \leq kd(x_1, x_0),
\]

\[
d(x_3, x_2) \leq kd(x_2, x_1) \leq k^2d(x_1, x_0),
\]

\[
\vdots
\]

\[
d(x_{n+1}, x_n) \leq kd(x_n, x_{n-1}) \leq \cdots \leq k^nd(x_1, x_0).
\]
Thus, we have
\[
d(x_{n+p}, x_n) \leq d(x_{n+p}, x_{n+p-1}) + d(x_{n+p-1}, x_{n+p-2}) + \cdots + d(x_{n+1}, x_n) \\
\leq (k^{p-1} + k^{p-2} + \cdots + k + 1)k^n d(x_1, x_0) \\
\leq \frac{k^n}{1-k} d(x_1, x_0).
\]

We conclude that \(d(x_{n+p}, x_n)\) converges to 0 when \(n\) goes to infinity, which shows that \((x_n)\) is a Cauchy sequence. Since \(E\) is complete, the sequence \((x_n)\) has a limit, \(a\). Since \(f\) is continuous, the sequence \((f(x_n))\) converges to \(f(a)\). But \(x_{n+1} = f(x_n)\) converges to \(a\) and so \(f(a) = a\), the unique fixed point of \(f\).

The above theorem is also called the Banach fixed point theorem. Note that no matter how the starting point \(x_0\) of the sequence \((x_n)\) is chosen, \((x_n)\) converges to the unique fixed point of \(f\). Also, the convergence is fast, since
\[
d(x_n, a) \leq \frac{k^n}{1-k} d(x_1, x_0).
\]

2.9 Further Readings

A thorough treatment of general topology can be found in Munkres [78, 77], Dixmier [35], Lang [66], Schwartz [91, 90], Bredon [23], and the classic, Seifert and Threlfall [95].

2.10 Summary

The main concepts and results of this chapter are listed below:

- Metric space, distance, metric.
- Euclidean metric, discrete metric.
- Closed ball, open ball, sphere, bounded subset.
- Normed vector space, norm.
- Open and closed sets.
- Topology, topological space.
- Hausdorff separation axiom, Hausdorff space.
- Discrete topology.
- Closure, dense subset, interior, frontier or boundary.
2.10. SUMMARY

- Subspace topology.
- Product topology.
- Basis of a topology, subbasis of a topology.
- Continuous functions.
- Neighborhood of a point.
- Homeomorphisms.
- Limits of sequences.
- Continuous linear maps.
- The norm of a continuous linear map.
- Continuous bilinear maps.
- The norm of a continuous bilinear map.
- The isomorphism between $\mathcal{L}(E, F; G)$ and $\mathcal{L}(E, \mathcal{L}(F; G))$.
- Cauchy sequences
- Complete metric spaces and Banach spaces.
- Completion of a metric space or of a normed vector space.
- Contractions.
- The contraction mapping theorem.
Chapter 3
Differential Calculus

3.1 Directional Derivatives, Total Derivatives

This chapter contains a review of basic notions of differential calculus. First, we review the
definition of the derivative of a function $f: \mathbb{R} \to \mathbb{R}$. Next, we define directional derivatives
and the total derivative of a function $f: E \to F$ between normed vector spaces. Basic
properties of derivatives are shown, including the chain rule. We show how derivatives
are represented by Jacobian matrices. The mean value theorem is stated, as well as the
implicit function theorem and the inverse function theorem. Diffeomorphisms and local
diffeomorphisms are defined. Higher-order derivatives are defined, as well as the Hessian.
Schwarz’s lemma (about the commutativity of partials) is stated. Several versions of Taylor’s
formula are stated, and a famous formula due to Faà di Bruno’s is given.

We first review the notion of the derivative of a real-valued function whose domain is an
open subset of $\mathbb{R}$.

Let $f: A \to \mathbb{R}$, where $A$ is a nonempty open subset of $\mathbb{R}$, and consider any $a \in A$.
The main idea behind the concept of the derivative of $f$ at $a$, denoted by $f'(a)$, is that
locally around $a$ (that is, in some small open set $U \subseteq A$ containing $a$), the function $f$
is approximated linearly\footnote{Actually, the approximation is affine, but everybody commits this abuse of language.} by the map

$$x \mapsto f(a) + f'(a)(x - a).$$

As pointed out by Dieudonné in the early 1960s, it is an “unfortunate accident” that if
$V$ is vector space of dimension one, then there is a bijection between the space $V^*$ of linear
forms defined on $V$ and the field of scalars. As a consequence, the derivative of a real-valued
function $f$ defined on an open subset $A$ of the reals can be defined as the scalar $f'(a)$ (for
any $a \in A$). But as soon as $f$ is a function of several arguments, the scalar interpretation of
the derivative breaks down.
Part of the difficulty in extending the idea of derivative to more complex spaces is to give an adequate notion of linear approximation. The key idea is to use linear maps. This could be carried out in terms of matrices but it turns out that this neither shortens nor simplifies proofs. In fact, this is often the opposite.

We admit that the more intrinsic definition of the notion of derivative $f'_a$ at a point $a$ of a function $f: E \to F$ between two normed vector spaces $E$ and $F$ as a linear map requires a greater effort to be grasped, but we feel that the advantages of this definition outweigh its degree of abstraction. In particular, it yields a clear notion of the derivative of a function $f: \mathbb{M}_m(\mathbb{R}) \to \mathbb{M}_n(\mathbb{R})$ defined from $m \times m$ matrices to $n \times n$ matrices (many definitions make use of partial derivatives with respect to matrices that do make any sense). But more importantly, the definition of the derivative as a linear map makes it clear that whether the space $E$ or the space $F$ is infinite dimensional does not matter. This is important in optimization theory where the natural space of solutions of the problem is often an infinite dimensional function space. Of course, to carry out computations one need to pick finite bases and to use Jacobian matrices, but this is a different matter.

Let us now review the formal definition of the derivative of a real-valued function.

**Definition 3.1.** Let $A$ be any nonempty open subset of $\mathbb{R}$, and let $a \in A$. For any function $f: A \to \mathbb{R}$, the derivative of $f$ at $a \in A$ is the limit (if it exists)

$$\lim_{h \to 0, h \in U} \frac{f(a + h) - f(a)}{h},$$

where $U = \{h \in \mathbb{R} | a + h \in A, h \neq 0\}$. This limit is denoted by $f'(a)$, or $Df(a)$, or $\frac{df}{dx}(a)$. If $f'(a)$ exists for every $a \in A$, we say that $f$ is differentiable on $A$. In this case, the map $a \mapsto f'(a)$ is denoted by $f'$, or $Df$, or $\frac{df}{dx}$.

Note that since $A$ is assumed to be open, $A - \{a\}$ is also open, and since the function $h \mapsto a + h$ is continuous and $U$ is the inverse image of $A - \{a\}$ under this function, $U$ is indeed open and the definition makes sense.

We can also define $f'(a)$ as follows: there is some function $\epsilon$, such that,

$$f(a + h) = f(a) + f'(a) \cdot h + \epsilon(h)h,$$

whenever $a + h \in A$, where $\epsilon(h)$ is defined for all $h$ such that $a + h \in A$, and

$$\lim_{h \to 0, h \in U} \epsilon(h) = 0.$$

**Remark:** We can also define the notion of derivative of $f$ at $a$ on the left, and derivative of $f$ at $a$ on the right. For example, we say that the derivative of $f$ at $a$ on the left is the limit $f'(a_\leftarrow)$ (if it exists)

$$f'(a_\leftarrow) = \lim_{h \to 0, h \in U} \frac{f(a + h) - f(a)}{h},$$
3.1. DIRECTIONAL DERIVATIVES, TOTAL DERIVATIVES

where \( U = \{ h \in \mathbb{R} \mid a + h \in A, h < 0 \} \).

If a function \( f \) as in Definition 20.1 has a derivative \( f'(a) \) at \( a \), then it is continuous at \( a \). If \( f \) is differentiable on \( A \), then \( f \) is continuous on \( A \). The composition of differentiable functions is differentiable.

**Remark:** A function \( f \) has a derivative \( f'(a) \) at \( a \) iff the derivative of \( f \) on the left at \( a \) and the derivative of \( f \) on the right at \( a \) exist, and if they are equal. Also, if the derivative of \( f \) on the left at \( a \) exists, then \( f \) is continuous on the left at \( a \) (and similarly on the right).

We would like to extend the notion of derivative to functions \( f : A \rightarrow F \), where \( E \) and \( F \) are normed vector spaces, and \( A \) is some nonempty open subset of \( E \). The first difficulty is to make sense of the quotient

\[
\frac{f(a + h) - f(a)}{h}.
\]

Since \( F \) is a normed vector space, \( f(a + h) - f(a) \) makes sense. But now, how do we define the quotient by a vector? Well, we don’t!

A first possibility is to consider the directional derivative with respect to a vector \( u \neq 0 \) in \( E \). We can consider the vector \( f(a + tu) - f(a) \), where \( t \in \mathbb{R} \). Now,

\[
\frac{f(a + tu) - f(a)}{t}
\]

makes sense.

The idea is that in \( E \), the points of the form \( a + tu \) for \( t \) in some small interval \([-\epsilon, +\epsilon] \) in \( \mathbb{R} \) form a line segment \([r, s] \) in \( A \) containing \( a \), and that the image of this line segment defines a small curve segment on \( f(A) \). This curve segment is defined by the map \( t \mapsto f(a + tu) \), from \([r, s] \) to \( F \), and the directional derivative \( D_u f(a) \) defines the direction of the tangent line at \( a \) to this curve; see Figure 20.1. This leads us to the following definition.

**Definition 3.2.** Let \( E \) and \( F \) be two normed vector spaces, let \( A \) be a nonempty open subset of \( E \), and let \( f : A \rightarrow F \) be any function. For any \( a \in A \), for any \( u \neq 0 \) in \( E \), the directional derivative of \( f \) at a w.r.t. the vector \( u \), denoted by \( D_u f(a) \), is the limit (if it exists)

\[
D_u f(a) = \lim_{t \rightarrow 0, t \in U} \frac{f(a + tu) - f(a)}{t},
\]

where \( U = \{ t \in \mathbb{R} \mid a + tu \in A, t \neq 0 \} \) (or \( U = \{ t \in \mathbb{C} \mid a + tu \in A, t \neq 0 \} \)).

Since the map \( t \mapsto a + tu \) is continuous, and since \( A - \{a\} \) is open, the inverse image \( U \) of \( A - \{a\} \) under the above map is open, and the definition of the limit in Definition 20.2 makes sense. The directional derivative is sometimes called the Gâteaux derivative.

**Remark:** Since the notion of limit is purely topological, the existence and value of a directional derivative is independent of the choice of norms in \( E \) and \( F \), as long as they are equivalent norms.
Figure 3.1: Let \( f : \mathbb{R}^2 \to \mathbb{R} \). The graph of \( f \) is the peach surface in \( \mathbb{R}^3 \), and \( t \mapsto f(a + tu) \) is the embedded orange curve connecting \( f(a) \) to \( f(a + tu) \). Then \( D_u f(a) \) is the slope of the pink tangent line in the direction of \( u \).

In the special case where \( E = \mathbb{R} \) and \( F = \mathbb{R} \), and we let \( u = 1 \) (i.e., the real number 1, viewed as a vector), it is immediately verified that \( D_1 f(a) = f'(a) \), in the sense of Definition 20.1. When \( E = \mathbb{R} \) (or \( E = \mathbb{C} \)) and \( F \) is any normed vector space, the derivative \( D_1 f(a) \), also denoted by \( f'(a) \), provides a suitable generalization of the notion of derivative.

However, when \( E \) has dimension \( \geq 2 \), directional derivatives present a serious problem, which is that their definition is not sufficiently uniform. Indeed, there is no reason to believe that the directional derivatives w.r.t. all nonnull vectors \( u \) share something in common. As a consequence, a function can have all directional derivatives at \( a \), and yet not be continuous at \( a \). Two functions may have all directional derivatives in some open sets, and yet their composition may not.

**Example 3.1.** Let \( f : \mathbb{R}^2 \to \mathbb{R} \) be the function given by

\[
f(x, y) = \begin{cases} 
\frac{x^2 y}{x^4 + y^2} & \text{if } (x, y) \neq (0, 0) \\
0 & \text{if } (x, y) = (0, 0).
\end{cases}
\]

For any \( u \neq 0 \), letting \( u = \left( \begin{array}{c} h \\ k \end{array} \right) \), we have

\[
\frac{f(0 + tu) - f(0)}{t} = \frac{h^2 k}{t^2 h^2 + k^2},
\]

so that

\[
D_u f(0, 0) = \begin{cases} 
\frac{h^2 k}{k} & \text{if } k \neq 0 \\
0 & \text{if } k = 0.
\end{cases}
\]
Thus, $D_u f(0,0)$ exists for all $u \neq 0$.

On the other hand, if $D_f(0,0)$ existed, it would be a linear map $D_f(0,0) : \mathbb{R}^2 \to \mathbb{R}$ represented by a row matrix $(\alpha \beta)$, and we would have $D_u f(0,0) = D_f(0,0)(u) = \alpha h + \beta k$, but the explicit formula for $D_u f(0,0)$ is not linear. As a matter of fact, the function $f$ is not continuous at $(0,0)$. For example, on the parabola $y = x^2$, $f(x,y) = \frac{1}{2}$, and when we approach the origin on this parabola, the limit is $\frac{1}{2}$, but $f(0,0) = 0$.

To avoid the problems arising with directional derivatives we introduce a more uniform notion.

Given two normed spaces $E$ and $F$, recall that a linear map $f : E \to F$ is continuous iff there is some constant $C \geq 0$ such that $\|f(u)\| \leq C \|u\|$ for all $u \in E$.

**Definition 3.3.** Let $E$ and $F$ be two normed vector spaces, let $A$ be a nonempty open subset of $E$, and let $f : A \to F$ be any function. For any $a \in A$, we say that $f$ is differentiable at $a \in A$ if there is a linear continuous map $L : E \to F$ and a function $h \mapsto \epsilon(h)$, such that

$$f(a+h) = f(a) + L(h) + \epsilon(h)\|h\|$$

for every $a+h \in A$, where $\epsilon(h)$ is defined for every $h$ such that $a+h \in A$, and

$$\lim_{h \to 0, h \in U} \epsilon(h) = 0,$$

where $U = \{h \in E \mid a+h \in A, h \neq 0\}$. The linear map $L$ is denoted by $Df(a)$, or $Df_a$, or $df(a)$, or $df_a$, or $f'(a)$, and it is called the Fréchet derivative, or derivative, or total derivative, or total differential, or differential, of $f$ at $a$; see Figure 20.2.

Since the map $h \mapsto a+h$ from $E$ to $E$ is continuous, and since $A$ is open in $E$, the inverse image $U$ of $A - \{a\}$ under the above map is open in $E$, and it makes sense to say that

$$\lim_{h \to 0, h \in U} \epsilon(h) = 0.$$ 

Note that for every $h \in U$, since $h \neq 0$, $\epsilon(h)$ is uniquely determined since

$$\epsilon(h) = \frac{f(a+h) - f(a) - L(h)}{\|h\|},$$

and that the value $\epsilon(0)$ plays absolutely no role in this definition. The condition for $f$ to be differentiable at $a$ amounts to the fact that

$$\lim_{h \to 0} \frac{\|f(a+h) - f(a) - L(h)\|}{\|h\|} = 0.$$
Figure 3.2: Let $f : \mathbb{R}^2 \to \mathbb{R}$. The graph of $f$ is the green surface in $\mathbb{R}^3$. The linear map $L = Df(a)$ is the pink tangent plane. For any vector $h \in \mathbb{R}^2$, $L(h)$ is approximately equal to $f(a + h) - f(a)$. Note that $L(h)$ is also the direction tangent to the curve $t \mapsto f(a + tu)$. as $h \neq 0$ approaches 0, when $a + h \in A$. However, it does no harm to assume that $\epsilon(0) = 0$, and we will assume this from now on.

Again, we note that the derivative $Df(a)$ of $f$ at $a$ provides an affine approximation of $f$, locally around $a$.

Remarks:

(1) Since the notion of limit is purely topological, the existence and value of a derivative is independent of the choice of norms in $E$ and $F$, as long as they are equivalent norms.

(2) If $h : (-a, a) \to \mathbb{R}$ is a real-valued function defined on some open interval containing 0, we say that $h$ is $o(t)$ for $t \to 0$, and we write $h(t) = o(t)$, if

$$\lim_{t \to 0, t \neq 0} \frac{h(t)}{t} = 0.$$ 

With this notation (the little o notation), the function $f$ is differentiable at $a$ iff

$$f(a + h) - f(a) - L(h) = o(\|h\|),$$

which is also written as

$$f(a + h) = f(a) + L(h) + o(\|h\|).$$
3.1. DIRECTIONAL DERIVATIVES, TOTAL DERIVATIVES

The following proposition shows that our new definition is consistent with the definition of the directional derivative and that the continuous linear map \( L \) is unique, if it exists.

**Proposition 3.1.** Let \( E \) and \( F \) be two normed spaces, let \( A \) be a nonempty open subset of \( E \), and let \( f : A \to F \) be any function. For any \( a \in A \), if \( Df(a) \) is defined, then \( f \) is continuous at \( a \) and \( f \) has a directional derivative \( Du f(a) \) for every \( u \neq 0 \) in \( E \). Furthermore,

\[
Du f(a) = Df(a)(u)
\]

and thus, \( Df(a) \) is uniquely defined.

**Proof.** If \( L = Df(a) \) exists, then for any nonzero vector \( u \in E \), because \( A \) is open, for any \( t \in \mathbb{R} - \{0\} \) (or \( t \in \mathbb{C} - \{0\} \)) small enough, \( a + tu \in A \), so

\[
f(a + tu) = f(a) + L(tu) + \epsilon(tu)\|tu\|
\]

which implies that

\[
L(u) = \frac{f(a + tu) - f(a)}{t} = \frac{|t|}{t} \epsilon(tu)\|u\|,
\]

and since \( \lim_{t \to 0} \epsilon(tu) = 0 \), we deduce that

\[
L(u) = Df(a)(u) = Du f(a).
\]

Because

\[
f(a + h) = f(a) + L(h) + \epsilon(h)\|h\|
\]

for all \( h \) such that \( \|h\| \) is small enough, \( L \) is continuous, and \( \lim_{h \to 0} \epsilon(h)\|h\| = 0 \), we have

\[
\lim_{h \to 0} f(a + h) = f(a),
\]

that is, \( f \) is continuous at \( a \).

When \( E \) is of finite dimension, every linear map is continuous (see Proposition 7.7 or Theorem 19.16), and this assumption is then redundant.

Although this may not be immediately obvious, the reason for requiring the linear map \( Df(a) \) to be continuous is to ensure that if a function \( f \) is differentiable at \( a \), then it is continuous at \( a \). This is certainly a desirable property of a differentiable function. In finite dimension this holds, but in infinite dimension this is not the case. The following proposition shows that if \( Df(a) \) exists at \( a \) and if \( f \) is continuous at \( a \), then \( Df(a) \) must be a continuous map. So if a function is differentiable at \( a \), then it is continuous iff the linear map \( Df(a) \) is continuous. We chose to include the second condition rather that the first in the definition of a differentiable function.

**Proposition 3.2.** Let \( E \) and \( F \) be two normed spaces, let \( A \) be a nonempty open subset of \( E \), and let \( f : A \to F \) be any function. For any \( a \in A \), if \( Df(a) \) is defined, then \( f \) is continuous at \( a \) iff \( Df(a) \) is a continuous linear map.
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Proof. Proposition 20.1 shows that if \( Df_a \) is defined and continuous then \( f \) is continuous at \( a \). Conversely, assume that \( Df_a \) exists and that \( f \) is continuous at \( a \). Since \( f \) is continuous at \( a \) and since \( Df_a \) exists, for any \( \eta > 0 \) there is some \( \rho \) with \( 0 < \rho < 1 \) such that if \( \| h \| \leq \rho \) then

\[
\| f(a + h) - f(a) \| \leq \frac{\eta}{2},
\]

and

\[
\| f(a + h) - f(a) - D_a(h) \| \leq \frac{\eta}{2} \| h \| \leq \frac{\eta}{2},
\]

so we have

\[
\| D_a(h) \| = \| D_a(h) - (f(a + h) - f(a)) + f(a + h) - f(a) \|
\]

\[
\leq \| f(a + h) - f(a) - D_a(h) \| + \| f(a + h) - f(a) \|
\]

\[
\leq \frac{\eta}{2} + \frac{\eta}{2} = \eta,
\]

which proves that \( Df_a \) is continuous at 0. By Proposition 19.14, \( Df_a \) is a continuous linear map.

As an example, consider the map \( f : M_n(\mathbb{R}) \to M_n(\mathbb{R}) \) given by

\[
f(A) = A^\top A - I,
\]

where \( M_n(\mathbb{R}) \) denotes the vector space of all \( n \times n \) matrices with real entries equipped with any matrix norm, since they are all equivalent; for example, pick the Frobenius norm \( \| A \|_F = \sqrt{\text{tr}(A^\top A)} \). We claim that

\[
Df(A)(H) = A^\top H + H^\top A, \quad \text{for all } A \text{ and } H \text{ in } M_n(\mathbb{R}).
\]

We have

\[
f(A + H) - f(A) - (A^\top H + H^\top A) = (A + H)^\top (A + H) - I - (A^\top A - I) - A^\top H - H^\top A
\]

\[
= A^\top A + A^\top H + H^\top A + H^\top H - A^\top A - A^\top H - H^\top A
\]

\[
= H^\top H.
\]

It follows that

\[
\epsilon(H) = \frac{f(A + H) - f(A) - (A^\top H + H^\top A)}{\| H \|} = \frac{H^\top H}{\| H \|},
\]

and since our norm is the Frobenius norm,

\[
\| \epsilon(H) \| = \left\| \frac{H^\top H}{\| H \|} \right\| \leq \frac{\| H^\top H \|}{\| H \|} = \| H^\top H \| = \| H \|,
\]

so

\[
\lim_{H \to 0} \epsilon(H) = 0,
\]
and we conclude that
\[ Df(A)(H) = A^\top H + H^\top A. \]

If \( Df(a) \) exists for every \( a \in A \), we get a map \( Df : A \to \mathcal{L}(E; F) \), called the \textit{derivative of} \( f \) \textit{on} \( A \), and also denoted by \( df \). Here \( \mathcal{L}(E; F) \) denotes the vector space of continuous linear maps from \( E \) to \( F \).

We now consider a number of standard results about derivatives. A function \( f : E \to F \) is said to be \textit{affine} if there is some linear map \( \overrightarrow{f} : E \to F \) and some fixed vector \( c \in F \), such that
\[ f(u) = \overrightarrow{f}(u) + c \]
for all \( u \in E \). We call \( \overrightarrow{f} \) the \textit{linear map associated with} \( f \).

\begin{proposition}
Given two normed spaces \( E \) and \( F \), if \( f : E \to F \) is a constant function, then \( Df(a) = 0 \), for every \( a \in E \). If \( f : E \to F \) is a continuous affine map, then \( Df(a) = \overrightarrow{f} \), for every \( a \in E \), where \( \overrightarrow{f} \) denotes the linear map associated with \( f \).
\end{proposition}

\begin{proposition}
Given a normed space \( E \) and a normed vector space \( F \), for any two functions \( f, g : E \to F \), for every \( a \in E \), if \( Df(a) \) and \( Dg(a) \) exist, then \( D(f + g)(a) \) and \( D(\lambda f)(a) \) exist, and
\[ D(f + g)(a) = Df(a) + Dg(a), \]
\[ D(\lambda f)(a) = \lambda Df(a). \]
\end{proposition}

Given two normed vector spaces \((E_1, \| \cdot \|_1)\) and \((E_2, \| \cdot \|_2)\), there are three natural and equivalent norms that can be used to make \( E_1 \times E_2 \) into a normed vector space:

1. \( \|(u_1, u_2)\|_1 = \|u_1\|_1 + \|u_2\|_2 \).
2. \( \|(u_1, u_2)\|_2 = (\|u_1\|_1^2 + \|u_2\|_2^2)^{1/2} \).
3. \( \|(u_1, u_2)\|_\infty = \max(\|u_1\|_1, \|u_2\|_2) \).

We usually pick the first norm. If \( E_1, E_2, \) and \( F \) are three normed vector spaces, recall that a bilinear map \( f : E_1 \times E_2 \to F \) is \textit{continuous} iff there is some constant \( C \geq 0 \) such that
\[ \|f(u_1, u_2)\| \leq C \|u_1\|_1 \|u_2\|_2 \quad \text{for all} \quad u_1 \in E_1 \text{ and all} \quad u_2 \in E_2. \]

\begin{proposition}
Given three normed vector spaces \( E_1, E_2, \) and \( F \), for any continuous bilinear map \( f : E_1 \times E_2 \to F \), for every \((a, b) \in E_1 \times E_2\), \( Df(a, b) \) exists, and for every \( u \in E_1 \) and \( v \in E_2 \),
\[ Df(a, b)(u, v) = f(u, b) + f(a, v). \]
\end{proposition}
Proof. Since $f$ is bilinear, a simple computation implies that

$$f((a, b) + (u, v)) - f(a, b) - (f(u, b) + f(a, v)) = f(a + u, b + v) - f(a, b) - f(u, b) - f(a, v)$$

$$= f(a + u, b) + f(a + u, v) - f(a, b) - f(u, b) - f(a, v)$$

$$= f(a, b) + f(u, b) + f(a, v) + f(u, v) - f(a, b) - f(u, b) - f(a, v)$$

$$= f(u, v).$$

We define

$$\epsilon(u, v) = \frac{f((a, b) + (u, v)) - f(a, b) - (f(u, b) + f(a, v))}{\| (u, v) \|_1},$$

and observe that the continuity of $f$ implies

$$\| f((a, b) + (u, v)) - f(a, b) - (f(u, b) + f(a, v)) \| = \| f(u, v) \|$$

$$\leq C \| u \|_1 \| v \|_2 \leq C (\| u \|_1 + \| v \|_2)^2.$$

Hence

$$\| \epsilon(u, v) \| = \left\| \frac{f(u, v)}{\| (u, v) \|_1} \right\| = \frac{\| f(u, v) \|}{\| (u, v) \|_1} \leq \frac{C (\| u \|_1 + \| v \|_2)^2}{\| u \|_1 + \| v \|_2} = C (\| u \|_1 + \| v \|_2) = C \| (u, v) \|_1,$$

which in turn implies

$$\lim_{(u, v) \to (0, 0)} \epsilon(u, v) = 0.$$

We now state the very useful chain rule.

Theorem 3.6. Given three normed spaces $E$, $F$, and $G$, let $A$ be an open set in $E$, and let $B$ an open set in $F$. For any functions $f : A \to F$ and $g : B \to G$, such that $f(A) \subseteq B$, for any $a \in A$, if $Df(a)$ exists and $Dg(f(a))$ exists, then $D(g \circ f)(a)$ exists, and

$$D(g \circ f)(a) = Dg(f(a)) \circ Df(a).$$

Proof. Since $f$ is differentiable at $a$ and $g$ is differentiable at $b = f(a)$ for every $\eta$ such that $0 < \eta < 1$ there is some $\rho > 0$ such that for all $s, t$, if $\| s \| \leq \rho$ and $\| t \| \leq \rho$ then

$$f(a + s) = f(a) + Df_a(s) + \epsilon_1(s)$$

$$g(b + t) = g(b) + Dg_b(t) + \epsilon_2(t),$$

with $\| \epsilon_1(s) \| \leq \eta \| s \|$ and $\| \epsilon_2(t) \| \leq \eta \| t \|$. Since $Df_a$ and $Dg_b$ are continuous, we have

$$\| Df_a(s) \| \leq \| Df_a \| \| s \|$$

and

$$\| Dg_b(t) \| \leq \| Dg_b \| \| t \|.$$


where, since \( \|\epsilon_1(s)\| \leq \eta \|s\| \) and \( \eta < 1 \), implies that
\[
\|Df_a(s) + \epsilon_1(s)\| \leq \|Df_a\| \|s\| + \|\epsilon_1(s)\| \leq \|Df_a\| \|s\| + \eta \|s\| \leq (\|Df_a\| + 1) \|s\|.
\]
Consequently, if \( \|s\| < \rho/(\|Df_a\| + 1) \), we have
\[
\|\epsilon_2(Df_a(s) + \epsilon_1(s))\| \leq \eta(\|Df_a\| + 1) \|s\|
\]
and
\[
\|Dg_b(\epsilon_1(s))\| \leq \|Dg_b\| \|\epsilon_1(s)\| \leq \eta \|Dg_b\| \|s\|.
\]
Then since \( b = f(a) \), using the above we have
\[
(g \circ f)(a + s) = g(f(a + s)) = g(b + Df_a(s) + \epsilon_1(s))
\]
\[
= g(b) + Dg_b(Df_a(s) + \epsilon_1(s)) + \epsilon_2(Df_a(s) + \epsilon_1(s))
\]
\[
= g(b) + (Dg_b \circ Df_a)(s) + Dg_b(\epsilon_1(s)) + \epsilon_2(Df_a(s) + \epsilon_1(s)).
\]
Now by \((*)_1\) and \((*)_2\) we have
\[
\|Dg_b(\epsilon_1(s)) + \epsilon_2(Df_a(s) + \epsilon_1(s))\| \leq \|Dg_b(\epsilon_1(s))\| + \|\epsilon_2(Df_a(s) + \epsilon_1(s))\|
\]
\[
\leq \eta \|Dg_b\| \|s\| + \eta(\|Df_a\| + 1) \|s\|
\]
\[
= \eta(\|Df_a\| + \|Dg_b\| + 1) \|s\|,
\]
so if we write \( \epsilon_3(s) = Dg_b(\epsilon_1(s)) + \epsilon_2(Df_a(s) + \epsilon_1(s)) \) we proved that
\[
(g \circ f)(a + s) = g(b) + (Dg_b \circ Df_a)(s) + \epsilon_3(s)
\]
with \( \epsilon_3(s) \leq \eta(\|Df_a\| + \|Dg_b\| + 1) \|s\| \), which proves that \( Dg_b \circ Df_a \) is the derivative of \( g \circ f \) at \( a \). Since \( Df_a \) and \( Dg_b \) are continuous, so is \( Dg_b \circ Df_a \), which proves our proposition. \( \square \)

Theorem 20.6 has many interesting consequences. We mention two corollaries.

**Proposition 3.7.** Given three normed vector spaces \( E, F, \) and \( G \), for any open subset \( A \) in \( E \), for any \( a \in A \), let \( f : A \to F \) such that \( Df(a) \) exists, and let \( g : F \to G \) be a continuous affine map. Then, \( D(g \circ f)(a) \) exists, and
\[
D(g \circ f)(a) = \overrightarrow{g} \circ Df(a),
\]
where \( \overrightarrow{g} \) is the linear map associated with the affine map \( g \).

**Proposition 3.8.** Given two normed vector spaces \( E \) and \( F \), let \( A \) be some open subset in \( E \), let \( B \) be some open subset in \( F \), let \( f : A \to B \) be a bijection from \( A \) to \( B \), and assume that \( Df \) exists on \( A \) and that \( Df^{-1} \) exists on \( B \). Then, for every \( a \in A \),
\[
Df^{-1}(f(a)) = (Df(a))^{-1}.
\]
Proposition 20.8 has the remarkable consequence that the two vector spaces \( E \) and \( F \) have the same dimension. In other words, a local property, the existence of a bijection \( f \) between an open set \( A \) of \( E \) and an open set \( B \) of \( F \), such that \( f \) is differentiable on \( A \) and \( f^{-1} \) is differentiable on \( B \), implies a global property, that the two vector spaces \( E \) and \( F \) have the same dimension.

Let us mention two more rules about derivatives that are used all the time.

Let \( \iota : \text{GL}(n, \mathbb{C}) \to M_n(\mathbb{C}) \) be the function (inversion) defined on invertible \( n \times n \) matrices by

\[
\iota(A) = A^{-1}.
\]

Observe that \( \text{GL}(n, \mathbb{C}) \) is indeed an open subset of the normed vector space \( M_n(\mathbb{C}) \) of complex \( n \times n \) matrices, since its complement is the closed set of matrices \( A \in M_n(\mathbb{C}) \) satisfying \( \det(A) = 0 \). Then we have

\[
d\iota_A(H) = -A^{-1}HA^{-1},
\]

for all \( A \in \text{GL}(n, \mathbb{C}) \) and for all \( H \in M_n(\mathbb{C}) \).

To prove the preceding line observe that for \( H \) with sufficiently small norm, we have

\[
\iota(A + H) - \iota(A) + A^{-1}HA^{-1} = (A + H)^{-1} - A^{-1} + A^{-1}HA^{-1}
\]

\[
= (A + H)^{-1}[I - (A + H)A^{-1} + (A + H)A^{-1}HA^{-1}]
\]

\[
= (A + H)^{-1}[I - I - HA^{-1} + HA^{-1} + HA^{-1}HA^{-1}]
\]

\[
= (A + H)^{-1}HA^{-1}HA^{-1}.
\]

Consequently, we get

\[
\epsilon(H) = \frac{\iota(A + H) - \iota(A) + A^{-1}HA^{-1}}{\|H\|} = \frac{(A + H)^{-1}HA^{-1}HA^{-1}}{\|H\|},
\]

and since

\[
\|(A + H)^{-1}HA^{-1}HA^{-1}\| \leq \|H\|^2 \|A^{-1}\|^2 \|(A + H)^{-1}\|,
\]

it is clear that \( \lim_{H \to 0} \epsilon(H) = 0 \), which proves that

\[
d\iota_A(H) = -A^{-1}HA^{-1}.
\]

In particular, if \( A = I \), then \( d\iota_I(H) = -H \).

Next, if \( f : M_n(\mathbb{C}) \to M_n(\mathbb{C}) \) and \( g : M_n(\mathbb{C}) \to M_n(\mathbb{C}) \) are differentiable matrix functions, then

\[
d(fg)_A(B) = df_A(B)g(A) + f(A)dg_A(B),
\]

for all \( A, B \in M_n(\mathbb{C}) \). This is known as the product rule.

When \( E \) is of finite dimension \( n \), for any basis, \((u_1, \ldots, u_n)\), of \( E \), we can define the directional derivatives with respect to the vectors in the basis \((u_1, \ldots, u_n)\) (actually, we can also do it for an infinite basis). This way we obtain the definition of partial derivatives, as follows:
Definition 3.4. For any two normed spaces $E$ and $F$, if $E$ is of finite dimension $n$, for every basis $(u_1, \ldots, u_n)$ for $E$, for every $a \in E$, for every function $f : E \to F$, the directional derivatives $D_{u_j}f(a)$ (if they exist) are called the partial derivatives of $f$ with respect to the basis $(u_1, \ldots, u_n)$. The partial derivative $D_{u_j}f(a)$ is also denoted by $\partial f / \partial x_j(a)$, or $\partial f / \partial x_j(a)$.

The notation $\partial f / \partial x_j(a)$ for a partial derivative, although customary and going back to Leibniz, is a “logical obscenity.” Indeed, the variable $x_j$ really has nothing to do with the formal definition. This is just another of these situations where tradition is just too hard to overthrow!

We now consider the situation where the normed vector space $F$ is a finite direct sum $F = F_1 \oplus \cdots \oplus F_m$.

Proposition 3.9. Given normed vector spaces $E$ and $F = F_1 \oplus \cdots \oplus F_m$, given any open subset $A$ of $E$, for any $a \in A$, for any function $f : A \to F$, letting $f = (f_1, \ldots, f_m)$, $Df(a)$ exists iff every $Df_i(a)$ exists, and

$$Df(a) = in_1 \circ Df_1(a) + \cdots + in_m \circ Df_m(a).$$

Proof. The proposition is a simple application of Theorem 20.6.

In the special case where $F$ is a normed vector space of finite dimension $m$, for any basis $(v_1, \ldots, v_m)$ of $F$, every vector $x \in F$ can be expressed uniquely as

$$x = x_1 v_1 + \cdots + x_m v_m,$$

where $(x_1, \ldots, x_m) \in K^m$, the coordinates of $x$ in the basis $(v_1, \ldots, v_m)$ (where $K = \mathbb{R}$ or $K = \mathbb{C}$). Thus, letting $F_i$ be the standard normed vector space $K$ with its natural structure, we note that $F$ is isomorphic to the direct sum $F = K \oplus \cdots \oplus K$. Then, every function $f : E \to F$ is represented by $m$ functions $(f_1, \ldots, f_m)$, where $f_i : E \to K$ (where $K = \mathbb{R}$ or $K = \mathbb{C}$), and

$$f(x) = f_1(x) v_1 + \cdots + f_m(x) v_m,$$

for every $x \in E$. The following proposition is an immediate corollary of Proposition 20.9.

Proposition 3.10. For any two normed vector spaces $E$ and $F$, if $F$ is of finite dimension $m$, for any basis $(v_1, \ldots, v_m)$ of $F$, a function $f : E \to F$ is differentiable at $a$ iff each $f_i$ is differentiable at $a$, and

$$Df(a)(u) = Df_1(a)(u)v_1 + \cdots + Df_m(a)(u)v_m,$$

for every $u \in E$. 
We now consider the situation where \( E \) is a finite direct sum. Given a normed vector space \( E = E_1 \oplus \cdots \oplus E_n \) and a normed vector space \( F \), given any open subset \( A \) of \( E \), for any \( c = (c_1, \ldots, c_n) \in A \), we define the continuous functions \( i_j^c : E_j \to E \), such that
\[
i_j^c(x) = (c_1, \ldots, c_{j-1}, x, c_{j+1}, \ldots, c_n).
\]
For any function \( f : A \to F \), we have functions \( f \circ i_j^c : E_j \to F \), defined on \( (i_j^c)^{-1}(A) \), which contains \( c_j \). If \( D(f \circ i_j^c)(c_j) \) exists, we call it the partial derivative of \( f \) w.r.t. its \( j \)th argument, at \( c \). We also denote this derivative by \( D_j f(c) \). Note that \( D_j f(c) \in \mathcal{L}(E_j; F) \).

This notion is a generalization of the notion defined in Definition 20.4. In fact, when \( E \) is of dimension \( n \), and a basis \( (u_1, \ldots, u_n) \) has been chosen, we can write \( E_i \oplus \cdots \oplus E_i \), for some obvious \( E_j \) (as explained just after Proposition 20.9), and then
\[
D_j f(c)(\lambda u_j) = \lambda \partial_j f(c),
\]
and the two notions are consistent. We will use freely the notation \( \partial_j f(c) \) instead of \( D_j f(c) \).

The notion \( \partial_j f(c) \) introduced in Definition 20.4 is really that of the vector derivative, whereas \( D_j f(c) \) is the corresponding linear map. Although perhaps confusing, we identify the two notions. The following proposition holds.

**Proposition 3.11.** Given a normed vector space \( E = E_1 \oplus \cdots \oplus E_n \), and a normed vector space \( F \), given any open subset \( A \) of \( E \), for any function \( f : A \to F \), for every \( c \in A \), if \( Df(c) \) exists, then each \( D_j f(c) \) exists, and
\[
Df(c)(u_1, \ldots, u_n) = D_1 f(c)(u_1) + \cdots + D_n f(c)(u_n),
\]
for every \( u_i \in E_i, 1 \leq i \leq n \). The same result holds for the finite product \( E_1 \times \cdots \times E_n \).

**Proof.** If \( i_j : E_j \to E \) is the linear map given by
\[
i_j(x) = (0, \ldots, 0, x, 0, \ldots, 0),
\]
then
\[
i_j^c(x) = (c_1, \ldots, c_{j-1}, 0, c_{j+1}, \ldots, c_n) + i_j(x),
\]
which shows that \( i_j^c \) is affine, so \( D_i^c j(x) = i_j \). The proposition is then a simple application of Theorem 20.6. \( \square \)

### 3.2 Jacobian Matrices

If both \( E \) and \( F \) are of finite dimension, for any basis \( (u_1, \ldots, u_n) \) of \( E \) and any basis \( (v_1, \ldots, v_m) \) of \( F \), every function \( f : E \to F \) is determined by \( m \) functions \( f_i : E \to \mathbb{R} \) (or \( f_i : E \to \mathbb{C} \)), where
\[
f(x) = f_1(x)v_1 + \cdots + f_m(x)v_m,
\]
3.2. JACOBIAN MATRICES

for every \( x \in E \). From Proposition 20.1, we have

\[
  Df(a)(u_j) = D_{u_j}f(a) = \partial_j f(a),
\]

and from Proposition 20.10, we have

\[
  Df(a)(u_j) = Df_1(a)(u_j)v_1 + \cdots + Df_i(a)(u_j)v_i + \cdots + Df_m(a)(u_j)v_m,
\]

that is,

\[
  Df(a)(u_j) = \partial_j f_1(a)v_1 + \cdots + \partial_j f_i(a)v_i + \cdots + \partial_j f_m(a)v_m.
\]

Since the \( j \)-th column of the \( m \times n \)-matrix representing \( Df(a) \) w.r.t. the bases \((u_1, \ldots, u_n)\) and \((v_1, \ldots, v_m)\) is equal to the components of the vector \( Df(a)(u_j) \) over the basis \((v_1, \ldots, v_m)\), the linear map \( Df(a) \) is determined by the \( m \times n \)-matrix \( J(f)(a) = (\partial_j f_i(a)) \), (or \( J(f)(a) = (\partial f_i/\partial x_j)(a) \)):

\[
  J(f)(a) = \begin{pmatrix}
    \partial_1 f_1(a) & \partial_2 f_1(a) & \cdots & \partial_n f_1(a) \\
    \partial_1 f_2(a) & \partial_2 f_2(a) & \cdots & \partial_n f_2(a) \\
    \vdots & \vdots & \ddots & \vdots \\
    \partial_1 f_m(a) & \partial_2 f_m(a) & \cdots & \partial_n f_m(a)
  \end{pmatrix}
\]

or

\[
  J(f)(a) = \begin{pmatrix}
    \partial f_1/\partial x_1(a) & \partial f_1/\partial x_2(a) & \cdots & \partial f_1/\partial x_n(a) \\
    \partial f_2/\partial x_1(a) & \partial f_2/\partial x_2(a) & \cdots & \partial f_2/\partial x_n(a) \\
    \vdots & \vdots & \ddots & \vdots \\
    \partial f_m/\partial x_1(a) & \partial f_m/\partial x_2(a) & \cdots & \partial f_m/\partial x_n(a)
  \end{pmatrix}
\]

This matrix is called the Jacobian matrix of \( Df \) at \( a \). When \( m = n \), the determinant, \( \det(J(f)(a)) \), of \( J(f)(a) \) is called the Jacobian of \( Df(a) \). From a previous remark, we know that this determinant in fact only depends on \( Df(a) \), and not on specific bases. However, partial derivatives give a means for computing it.

When \( E = \mathbb{R}^n \) and \( F = \mathbb{R}^m \), for any function \( f: \mathbb{R}^n \to \mathbb{R}^m \), it is easy to compute the partial derivatives \( (\partial f_i/\partial x_j)(a) \). We simply treat the function \( f_i: \mathbb{R}^n \to \mathbb{R} \) as a function of its \( j \)-th argument, leaving the others fixed, and compute the derivative as in Definition 20.1, that is, the usual derivative.

**Example 3.2.** For example, consider the function \( f: \mathbb{R}^2 \to \mathbb{R}^2 \), defined such that

\[
  f(r, \theta) = (r \cos(\theta), r \sin(\theta)).
\]

Then, we have

\[
  J(f)(r, \theta) = \begin{pmatrix}
    \cos(\theta) & -r \sin(\theta) \\
    \sin(\theta) & r \cos(\theta)
  \end{pmatrix}
\]

and the Jacobian (determinant) has value \( \det(J(f)(r, \theta)) = r \).
In the case where \( E = \mathbb{R} \) (or \( E = \mathbb{C} \)), for any function \( f: \mathbb{R} \to F \) (or \( f: \mathbb{C} \to F \)), the Jacobian matrix of \( Df(a) \) is a column vector. In fact, this column vector is just \( D_1 f(a) \). Then, for every \( \lambda \in \mathbb{R} \) (or \( \lambda \in \mathbb{C} \)),

\[
Df(a)(\lambda) = \lambda D_1 f(a).
\]

This case is sufficiently important to warrant a definition.

**Definition 3.5.** Given a function \( f: \mathbb{R} \to F \) (or \( f: \mathbb{C} \to F \)), where \( F \) is a normed vector space, the vector \( Df(a)(1) = D_1 f(a) \) is called the **vector derivative or velocity vector (in the real case)** at \( a \). We usually identify \( Df(a) \) with its Jacobian matrix \( D_1 f(a) \), which is the column vector corresponding to \( D_1 f(a) \). By abuse of notation, we also let \( Df(a) \) denote the vector \( Df(a)(1) = D_1 f(a) \).

When \( E = \mathbb{R} \), the physical interpretation is that \( f \) defines a (parametric) curve that is the trajectory of some particle moving in \( \mathbb{R}^m \) as a function of time, and the vector \( D_1 f(a) \) is the velocity of the moving particle \( f(t) \) at \( t = a \); see Figure 20.3.

It is often useful to consider functions \( f: [a, b] \to F \) from a closed interval \( [a, b] \subseteq \mathbb{R} \) to a normed vector space \( F \), and its derivative \( Df(a) \) on \( [a, b] \), even though \( [a, b] \) is not open. In this case, as in the case of a real-valued function, we define the right derivative \( D_1 f(a_+) \) at \( a \), and the left derivative \( D_1 f(b_-) \) at \( b \), and we assume their existence.

**Example 3.3.**

1. When \( A = (0, 1) \) and \( F = \mathbb{R}^3 \), a function \( f: (0, 1) \to \mathbb{R}^3 \) defines a (parametric) curve in \( \mathbb{R}^3 \). If \( f = (f_1, f_2, f_3) \), its Jacobian matrix at \( a \in \mathbb{R} \) is

\[
J(f)(a) = \begin{pmatrix}
\frac{\partial f_1}{\partial t}(a) \\
\frac{\partial f_2}{\partial t}(a) \\
\frac{\partial f_3}{\partial t}(a)
\end{pmatrix}.
\]

See Figure 20.3.

The velocity vectors \( J(f)(a) = \begin{pmatrix} -\sin(t) \\ \cos(t) \\ 1 \end{pmatrix} \) are represented by the blue arrows.
2. When $E = \mathbb{R}^2$ and $F = \mathbb{R}^3$, a function $\varphi: \mathbb{R}^2 \to \mathbb{R}^3$ defines a parametric surface. Letting $\varphi = (f, g, h)$, its Jacobian matrix at $a \in \mathbb{R}^2$ is

$$J(\varphi)(a) = \begin{pmatrix} \frac{\partial f}{\partial u}(a) & \frac{\partial f}{\partial v}(a) \\ \frac{\partial g}{\partial u}(a) & \frac{\partial g}{\partial v}(a) \\ \frac{\partial h}{\partial u}(a) & \frac{\partial h}{\partial v}(a) \end{pmatrix}. $$

See Figure 20.4. The Jacobian matrix is $J(f)(a) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 2u & 2v \end{pmatrix}$. The first column is the vector tangent to the pink $u$-direction curve, while the second column is the vector tangent to the blue $v$-direction curve.

3. When $E = \mathbb{R}^3$ and $F = \mathbb{R}$, for a function $f: \mathbb{R}^3 \to \mathbb{R}$, the Jacobian matrix at $a \in \mathbb{R}^3$ is

$$J(f)(a) = \begin{pmatrix} \frac{\partial f}{\partial x_1}(a) & \cdots & \frac{\partial f}{\partial x_n}(a) \end{pmatrix}. $$

More generally, when $f: \mathbb{R}^n \to \mathbb{R}$, the Jacobian matrix at $a \in \mathbb{R}^n$ is the row vector

$$J(f)(a) = \begin{pmatrix} \frac{\partial f}{\partial x_1}(a) \\ \vdots \\ \frac{\partial f}{\partial x_n}(a) \end{pmatrix}. $$

Its transpose is a column vector called the gradient of $f$ at $a$, denoted by $\text{grad} f(a)$ or $\nabla f(a)$. Then, given any $v \in \mathbb{R}^n$, note that

$$Df(a)(v) = \frac{\partial f}{\partial x_1}(a) v_1 + \cdots + \frac{\partial f}{\partial x_n}(a) v_n = \text{grad} f(a) \cdot v,$$
the scalar product of $\text{grad} f(a)$ and $v$.

**Example 3.4.** Consider the quadratic function $f : \mathbb{R}^n \to \mathbb{R}$ given by

$$f(x) = x^\top Ax, \quad x \in \mathbb{R}^n,$$

where $A$ is a real $n \times n$ symmetric matrix. We claim that

$$df_u(h) = 2u^\top Ah \quad \text{for all } u, h \in \mathbb{R}^n.$$

Since $A$ is symmetric, we have

$$f(u + h) = (u^\top + h^\top)A(u + h)$$
$$= u^\top Au + u^\top Ah + h^\top Au + h^\top Ah$$
$$= u^\top Au + 2u^\top Ah + h^\top Ah,$$

so we have

$$f(u + h) - f(u) - 2u^\top Ah = h^\top Ah.$$

If we write

$$\epsilon(h) = \frac{h^\top Ah}{\|h\|}$$

for $h \notin 0$ where $\| \|$ is the 2-norm, by Cauchy–Schwarz we have

$$|\epsilon(h)| \leq \frac{\|h\| \|Ah\|}{\|h\|} \leq \frac{\|h\|^2 \|A\|}{\|h\|} = \|h\| \|A\|,$$
which shows that \( \lim_{h \to 0} \epsilon(h) = 0 \). Therefore, \[ df_u(h) = 2u^\top Ah \] for all \( u, h \in \mathbb{R}^n \), as claimed. This formula shows that the gradient \( \nabla f_u \) of \( f \) at \( u \) is given by \[ \nabla f_u = 2Au. \]

As a first corollary we obtain the gradient of a function of the form
\[ f(x) = \frac{1}{2} x^\top Ax - b^\top x, \]
where \( A \) is a symmetric \( n \times n \) matrix and \( b \) is some vector \( b \in \mathbb{R}^n \). Since the derivative of a linear function is itself, we obtain
\[ df_u(h) = u^\top Ah - b^\top h, \]
and the gradient of \( f \) is given by \[ \nabla f_u = Au - b. \]

As a second corollary we obtain the gradient of the function
\[ f(x) = \|Ax - b\|^2_2 = (Ax - b)^\top (Ax - b) = (x^\top A^\top - b^\top)(Ax - b) \]
which is the function to minimize in a least squares problem, where \( A \) is an \( m \times n \) matrix. We have
\[ f(x) = x^\top A^\top Ax - x^\top A^\top b - b^\top Ax + b^\top b = x^\top A^\top Ax - 2b^\top Ax + b^\top b, \]
and since the derivative of a constant function is 0 and the derivative of a linear function is itself, we get
\[ df_u(h) = 2u^\top A^\top Ah - 2b^\top Ah. \]
Consequently, the gradient of \( f \) is given by
\[ \nabla f_u = 2A^\top Au - 2A^\top b. \]

When \( E, F, \) and \( G \) have finite dimensions, and \( (u_1, \ldots, u_p) \) is a basis for \( E \), \( (v_1, \ldots, v_n) \) is a basis for \( F \), and \( (w_1, \ldots, w_m) \) is a basis for \( G \), if \( A \) is an open subset of \( E \), \( B \) is an open subset of \( F \), for any functions \( f: A \to F \) and \( g: B \to G \), such that \( f(A) \subseteq B \), for any \( a \in A \), letting \( b = f(a) \), and \( h = g \circ f \), if \( Df(a) \) exists and \( Dg(b) \) exists, by Theorem 20.6, the Jacobian matrix \( J(h)(a) = J(g \circ f)(a) \) w.r.t. the bases \( (u_1, \ldots, u_p) \) and \( (w_1, \ldots, w_m) \) is
the product of the Jacobian matrices $J(g)(b)$ w.r.t. the bases $(v_1, \ldots, v_n)$ and $(w_1, \ldots, w_m)$, and $J(f)(a)$ w.r.t. the bases $(u_1, \ldots, u_p)$ and $(v_1, \ldots, v_n)$:

$$J(h)(a) = \begin{pmatrix} \frac{\partial g_1}{\partial y_1} & \frac{\partial g_1}{\partial y_2} & \cdots & \frac{\partial g_1}{\partial y_n} \\ \frac{\partial g_2}{\partial y_1} & \frac{\partial g_2}{\partial y_2} & \cdots & \frac{\partial g_2}{\partial y_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial g_m}{\partial y_1} & \frac{\partial g_m}{\partial y_2} & \cdots & \frac{\partial g_m}{\partial y_n} \end{pmatrix} \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_p} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \cdots & \frac{\partial f_2}{\partial x_p} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_n}{\partial x_1} & \frac{\partial f_n}{\partial x_2} & \cdots & \frac{\partial f_n}{\partial x_p} \end{pmatrix}\frac{\partial h}{\partial y_k}(a) \frac{\partial \overline{g_i}}{\partial x_j}(a).

Thus, we have the familiar formula

$$\frac{\partial h_i}{\partial x_j}(a) = \sum_{k=1}^{k=n} \frac{\partial g_i}{\partial y_k}(a) \frac{\partial f_k}{\partial x_j}(a).$$

Given two normed vector spaces $E$ and $F$ of finite dimension, given an open subset $A$ of $E$, if a function $f: A \to F$ is differentiable at $a \in A$, then its Jacobian matrix is well defined. One should be warned that the converse is false. There are functions such that all the partial derivatives exist at some $a \in A$, but yet, the function is not differentiable at $a$, and not even continuous at $a$. For example, consider the function $f: \mathbb{R}^2 \to \mathbb{R}$, defined such that $f(0, 0) = 0$, and

$$f(x, y) = \frac{x^2 y}{x^4 + y^2} \quad \text{if } (x, y) \neq (0, 0).$$

For any $u \neq 0$, letting $u = \begin{pmatrix} h \\ k \end{pmatrix}$, we have

$$\frac{f(0 + tu) - f(0)}{t} = \frac{h^2 k}{t^2 h^4 + k^2},$$

so that

$$D_u f(0, 0) = \begin{cases} \frac{h^2}{k} & \text{if } k \neq 0 \\ 0 & \text{if } k = 0. \end{cases}$$

Thus, $D_u f(0, 0)$ exists for all $u \neq 0$. On the other hand, if $D f(0, 0)$ existed, it would be a linear map $D f(0, 0): \mathbb{R}^2 \to \mathbb{R}$ represented by a row matrix $\begin{pmatrix} \alpha & \beta \end{pmatrix}$, and we would have
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\[ D_u f(0,0) = D f(0,0)(u) = \alpha h + \beta k, \] but the explicit formula for \( D_u f(0,0) \) is not linear. As a matter of fact, the function \( f \) is not continuous at \((0,0)\). For example, on the parabola \( y = x^2 \), \( f(x,y) = \frac{x}{2} \), and when we approach the origin on this parabola, the limit is \( \frac{1}{2} \), when in fact, \( f(0,0) = 0 \).

However, there are sufficient conditions on the partial derivatives for \( D f(a) \) to exist, namely, continuity of the partial derivatives.

If \( f \) is differentiable on \( A \), then \( f \) defines a function \( D f : A \to \mathcal{L}(E;F) \). It turns out that the continuity of the partial derivatives on \( A \) is a necessary and sufficient condition for \( D f \) to exist and to be continuous on \( A \).

If \( f : [a,b] \to \mathbb{R} \) is a function which is continuous on \([a,b]\) and differentiable on \( ]a,b] \), then there is some \( c \) with \( a < c < b \) such that

\[ f(b) - f(a) = (b - a)f'(c). \]

This result is known as the mean value theorem and is a generalization of Rolle’s theorem, which corresponds to the case where \( f(a) = f(b) \).

Unfortunately, the mean value theorem fails for vector-valued functions. For example, the function \( f : [0, 2\pi] \to \mathbb{R}^2 \) given by

\[ f(t) = (\cos t, \sin t) \]

is such that \( f(2\pi) - f(0) = (0,0) \), yet its derivative \( f'(t) = (-\sin t, \cos t) \) does not vanish in \((0, 2\pi)\).

A suitable generalization of the mean value theorem to vector-valued functions is possible if we consider an inequality (an upper bound) instead of an equality. This generalized version of the mean value theorem plays an important role in the proof of several major results of differential calculus.

If \( E \) is an vector space (over \( \mathbb{R} \) or \( \mathbb{C} \)), given any two points \( a, b \in E \), the closed segment \([a,b]\) is the set of all points \( a + \lambda(b - a) \), where \( 0 \leq \lambda \leq 1 \), \( \lambda \in \mathbb{R} \), and the open segment \((a,b)\) is the set of all points \( a + \lambda(b - a) \), where \( 0 < \lambda < 1 \), \( \lambda \in \mathbb{R} \).

**Lemma 3.12.** Let \( E \) and \( F \) be two normed vector spaces, let \( A \) be an open subset of \( E \), and let \( f : A \to F \) be a continuous function on \( A \). Given any \( a \in A \) and any \( h \neq 0 \) in \( E \), if the closed segment \([a,a+h]\) is contained in \( A \), if \( f : A \to F \) is differentiable at every point of the open segment \((a,a+h)\), and

\[ \sup_{x \in (a,a+h)} \|Df(x)\| \leq M, \]

for some \( M \geq 0 \), then

\[ \|f(a+h) - f(a)\| \leq M\|h\|. \]
As a corollary, if \( L: E \to F \) is a continuous linear map, then
\[
\| f(a + h) - f(a) - L(h) \| \leq M \| h \|
\]
where \( M = \sup_{x \in (a, a + h)} \| Df(x) - L \| \).

The above lemma is sometimes called the “mean value theorem.” Lemma 20.12 can be used to show the following important result.

**Theorem 3.13.** Given two normed vector spaces \( E \) and \( F \), where \( E \) is of finite dimension \( n \), and where \((u_1, \ldots, u_n)\) is a basis of \( E \), given any open subset \( A \) of \( E \), given any function \( f: A \to F \), the derivative \( Df: A \to \mathcal{L}(E; F) \) is defined and continuous on \( A \) iff every partial derivative \( \partial_j f \) (or \( \frac{\partial f}{\partial x_j} \)) is defined and continuous on \( A \), for all \( j, 1 \leq j \leq n \). As a corollary, if \( F \) is of finite dimension \( m \), and \((v_1, \ldots, v_m)\) is a basis of \( F \), the derivative \( Df: A \to \mathcal{L}(E; F) \) is defined and continuous on \( A \) iff every partial derivative \( \partial_j f_i \) (or \( \frac{\partial f_i}{\partial x_j} \)) is defined and continuous on \( A \), for all \( i, j, 1 \leq i \leq m, 1 \leq j \leq n \).

Theorem 20.13 gives a necessary and sufficient condition for the existence and continuity of the derivative of a function on an open set. It should be noted that a more general version of Theorem 20.13 holds, assuming that \( E = E_1 \oplus \cdots \oplus E_n \), or \( E = E_1 \times \cdots \times E_n \), and using the more general partial derivatives \( D_j f \) introduced before Proposition 20.11.

**Definition 3.6.** Given two normed vector spaces \( E \) and \( F \), and an open subset \( A \) of \( E \), we say that a function \( f: A \to F \) is of class \( C^0 \) on \( A \) or a \( C^0 \)-function on \( A \) if \( f \) is continuous on \( A \). We say that \( f: A \to F \) is of class \( C^1 \) on \( A \) or a \( C^1 \)-function on \( A \) if \( Df \) exists and is continuous on \( A \).

Since the existence of the derivative on an open set implies continuity, a \( C^1 \)-function is of course a \( C^0 \)-function. Theorem 20.13 gives a necessary and sufficient condition for a function \( f \) to be a \( C^1 \)-function (when \( E \) is of finite dimension). It is easy to show that the composition of \( C^1 \)-functions (on appropriate open sets) is a \( C^1 \)-function.

### 3.3 The Implicit and The Inverse Function Theorems

Given three normed vector spaces \( E, F, \) and \( G \), given a function \( f: E \times F \to G \), given any \( c \in G \), it may happen that the equation
\[
f(x, y) = c
\]
has the property that, for some open sets \( A \subseteq E \), and \( B \subseteq F \), there is a function \( g: A \to B \), such that
\[
f(x, g(x)) = c,
\]
for all \( x \in A \). Such a situation is usually very rare, but if some solution \((a, b) \in E \times F\) such that \( f(a, b) = c \) is known, under certain conditions, for some small open sets \( A \subseteq E \) containing \( a \) and \( B \subseteq F \) containing \( b \), the existence of a unique \( g : A \to B \), such that

\[
f(x, g(x)) = c,
\]

for all \( x \in A \), can be shown. Under certain conditions, it can also be shown that \( g \) is continuous, and differentiable. Such a theorem, known as the *implicit function theorem*, can be shown. We state a version of this result below. The proof is fairly involved, and uses a fixed-point theorem for contracting mappings in complete metric spaces; it is given in Schwartz [92].

**Theorem 3.14.** Let \( E, F, \) and \( G \), be normed vector spaces, let \( \Omega \) be an open subset of \( E \times F \), let \( f : \Omega \to G \) be a function defined on \( \Omega \), let \((a, b) \in \Omega \), let \( c \in G \), and assume that \( f(a, b) = c \). If the following assumptions hold:

1. The function \( f : \Omega \to G \) is continuous on \( \Omega \);
2. \( F \) is a complete normed vector space (and so is \( G \));
3. \( \frac{\partial f}{\partial y}(x, y) \) exists for every \((x, y) \in \Omega\), and \( \frac{\partial f}{\partial y} : \Omega \to \mathcal{L}(F; G) \) is continuous;
4. \( \frac{\partial f}{\partial y}(a, b) \) is a bijection of \( \mathcal{L}(F; G) \), and \( \left( \frac{\partial f}{\partial y}(a, b) \right)^{-1} \in \mathcal{L}(G; F) \);

then the following properties hold:

1. There exist some open subset \( A \subseteq E \) containing \( a \) and some open subset \( B \subseteq F \) containing \( b \), such that \( A \times B \subseteq \Omega \), and for every \( x \in A \), the equation \( f(x, y) = c \) has a single solution \( y = g(x) \), and thus, there is a unique function \( g : A \to B \) such that \( f(x, g(x)) = c \), for all \( x \in A \);
2. The function \( g : A \to B \) is continuous.

If we also assume that

5. The derivative \( Df(a, b) \) exists;

then

1. The derivative \( Dg(a) \) exists, and

\[
Dg(a) = -\left( \frac{\partial f}{\partial y}(a, b) \right)^{-1} \circ \frac{\partial f}{\partial x}(a, b);
\]

and if in addition
(6) \( \frac{\partial f}{\partial x} : \Omega \to \mathcal{L}(E; G) \) is also continuous (and thus, in view of (3), \( f \) is \( C^1 \) on \( \Omega \));

then

(d) The derivative \( Dg : A \to \mathcal{L}(E; F) \) is continuous, and

\[
Dg(x) = -\left( \frac{\partial f}{\partial y}(x, g(x)) \right)^{-1} \circ \frac{\partial f}{\partial x}(x, g(x)),
\]

for all \( x \in A \).

The implicit function theorem plays an important role in the calculus of variations. We now consider another very important notion, that of a (local) diffeomorphism.

**Definition 3.7.** Given two topological spaces \( E \) and \( F \), and an open subset \( A \) of \( E \), we say that a function \( f : A \to F \) is a local homeomorphism from \( A \) to \( F \) if for every \( a \in A \), there is an open set \( U \subseteq A \) containing \( a \) and an open set \( V \) containing \( f(a) \) such that \( f \) is a homeomorphism from \( U \) to \( V = f(U) \). If \( B \) is an open subset of \( F \), we say that \( f : A \to F \) is a (global) homeomorphism from \( A \) to \( B = f(A) \). If \( E \) and \( F \) are normed vector spaces, we say that \( f : A \to F \) is a local diffeomorphism from \( A \) to \( F \) if for every \( a \in A \), there is an open set \( U \subseteq A \) containing \( a \) and an open set \( V \) containing \( f(a) \) such that \( f \) is a bijection from \( U \) to \( V \), \( f \) is a \( C^1 \)-function on \( U \), and \( f^{-1} \) is a \( C^1 \)-function on \( V = f(U) \). We say that \( f : A \to F \) is a (global) diffeomorphism from \( A \) to \( B \) if \( f \) is a homeomorphism from \( A \) to \( B = f(A) \), \( f \) is a \( C^1 \)-function on \( A \), and \( f^{-1} \) is a \( C^1 \)-function on \( B \).

Note that a local diffeomorphism is a local homeomorphism. Also, as a consequence of Proposition 20.8, if \( f \) is a diffeomorphism on \( A \), then \( Df(a) \) is a bijection for every \( a \in A \). The following theorem can be shown. In fact, there is a fairly simple proof using Theorem 20.14.

**Theorem 3.15.** (Inverse Function Theorem) Let \( E \) and \( F \) be complete normed spaces, let \( A \) be an open subset of \( E \), and let \( f : A \to F \) be a \( C^1 \)-function on \( A \). The following properties hold:

(1) For every \( a \in A \), if \( Df(a) \) is a linear isomorphism (which means that both \( Df(a) \) and \( (Df(a))^{-1} \) are linear and continuous),\(^2\) then there exist some open subset \( U \subseteq A \) containing \( a \), and some open subset \( V \) of \( F \) containing \( f(a) \), such that \( f \) is a diffeomorphism from \( U \) to \( V = f(U) \). Furthermore,

\[
Df^{-1}(f(a)) = (Df(a))^{-1}.
\]

For every neighborhood \( N \) of \( a \), the image \( f(N) \) of \( N \) is a neighborhood of \( f(a) \), and for every open ball \( U \subseteq A \) of center \( a \), the image \( f(U) \) of \( U \) contains some open ball of center \( f(a) \).

\(^2\) Actually, since \( E \) and \( F \) are Banach spaces, by the Open Mapping Theorem, it is sufficient to assume that \( Df(a) \) is continuous and bijective; see Lang [65].
(2) If $Df(a)$ is invertible for every $a \in A$, then $B = f(A)$ is an open subset of $F$, and $f$ is a local diffeomorphism from $A$ to $B$. Furthermore, if $f$ is injective, then $f$ is a diffeomorphism from $A$ to $B$.

Proofs of the Inverse function theorem can be found in Lang [65], Abraham and Marsden [1], Schwartz [92], and Cartan [26]. Part (1) of Theorem 20.15 is often referred to as the “(local) inverse function theorem.” It plays an important role in the study of manifolds and (ordinary) differential equations.

If $E$ and $F$ are both of finite dimension, and some bases have been chosen, the invertibility of $Df(a)$ is equivalent to the fact that the Jacobian determinant $\det(J(f)(a))$ is nonnull. The case where $Df(a)$ is just injective or just surjective is also important for defining manifolds, using implicit definitions.

**Definition 3.8.** Let $E$ and $F$ be normed vector spaces, where $E$ and $F$ are of finite dimension (or both $E$ and $F$ are complete), and let $A$ be an open subset of $E$. For any $a \in A$, a $C^1$-function $f : A \to F$ is an **immersion at** $a$ if $Df(a)$ is injective. A $C^1$-function $f : A \to F$ is a **submersion at** $a$ if $Df(a)$ is surjective. A $C^1$-function $f : A \to F$ is an **immersion on** $A$ (resp. a **submersion on** $A$) if $Df(a)$ is injective (resp. surjective) for every $a \in A$.

When $E$ and $F$ are finite dimensional with $\dim(E) = n$ and $\dim(F) = m$, if $m \geq n$, then $f$ is an immersion iff the Jacobian matrix, $J(f)(a)$, has full rank $n$ for all $a \in E$ and if $n \geq m$, then $f$ is a submersion iff the Jacobian matrix, $J(f)(a)$, has full rank $m$ for all $a \in E$. For example, $f : \mathbb{R} \to \mathbb{R}^2$ defined by $f(t) = (\cos(t), \sin(t))$ is an immersion since $J(f)(t) = \begin{pmatrix} -\sin(t) \\ \cos(t) \end{pmatrix}$ has rank 1 for all $t$. On the other hand, $f : \mathbb{R} \to \mathbb{R}^2$ defined by $f(t) = (t^2, t^2)$ is not an immersion since $J(f)(t) = \begin{pmatrix} 2t \\ 2t \end{pmatrix}$ vanishes at $t = 0$. See Figure 20.5.

An example of a submersion is given by the projection map $f : \mathbb{R}^2 \to \mathbb{R}$, where $f(x, y) = x$, since $J(f)(x, y) = (1 \ 0)$.

The following results can be shown.

**Proposition 3.16.** Let $A$ be an open subset of $\mathbb{R}^n$, and let $f : A \to \mathbb{R}^m$ be a function. For every $a \in A$, $f : A \to \mathbb{R}^m$ is a submersion at $a$ iff there exists an open subset $U$ of $A$ containing $a$, an open subset $W \subseteq \mathbb{R}^{n-m}$, and a diffeomorphism $\varphi : U \to f(U) \times W$, such that,

$$f = \pi_1 \circ \varphi,$$

where $\pi_1 : f(U) \times W \to f(U)$ is the first projection. Equivalently,

$$(f \circ \varphi^{-1})(y_1, \ldots, y_m, \ldots, y_n) = (y_1, \ldots, y_m).$$

\[ U \subseteq A \xrightarrow{\varphi} f(U) \times W \xrightarrow{\pi_1} f(U) \subseteq \mathbb{R}^m \]
Figure 3.5: Figure (i.) is the immersion of \( \mathbb{R} \) into \( \mathbb{R}^2 \) given by \( f(t) = (\cos(t), \sin(t)) \). Figure (ii.), the parametric curve \( f(t) = (t^2, t^2) \), is not an immersion since the tangent vanishes at the origin.

Furthermore, the image of every open subset of \( A \) under \( f \) is an open subset of \( F \). (The same result holds for \( \mathbb{C}^n \) and \( \mathbb{C}^m \)).

**Proposition 3.17.** Let \( A \) be an open subset of \( \mathbb{R}^n \), and let \( f: A \to \mathbb{R}^m \) be a function. For every \( a \in A \), \( f: A \to \mathbb{R}^m \) is an immersion at \( a \) iff there exists an open subset \( U \) of \( A \) containing \( a \), an open subset \( V \) containing \( f(a) \) such that \( f(U) \subseteq V \), an open subset \( W \) containing \( 0 \) such that \( W \subseteq \mathbb{R}^{m-n} \), and a diffeomorphism \( \varphi: V \to U \times W \), such that,

\[
\varphi \circ f = \text{in}_1,
\]

where \( \text{in}_1: U \to U \times W \) is the injection map such that \( \text{in}_1(u) = (u, 0) \), or equivalently,

\[
(\varphi \circ f)(x_1, \ldots, x_n) = (x_1, \ldots, x_n, 0, \ldots, 0).
\]

\[
\begin{align*}
U \subseteq A & \xrightarrow{f} f(U) \subseteq V \\
& \xrightarrow{\text{in}_1} U \times W \\
& \xrightarrow{\varphi} \end{align*}
\]

(The same result holds for \( \mathbb{C}^n \) and \( \mathbb{C}^m \)).

We now briefly consider second-order and higher-order derivatives.
3.4 Second-Order and Higher-Order Derivatives

Given two normed vector spaces $E$ and $F$, and some open subset $A$ of $E$, if $Df(a)$ is defined for every $a \in A$, then we have a mapping $Df: A \to \mathcal{L}(E; F)$. Since $\mathcal{L}(E; F)$ is a normed vector space, if $Df$ exists on an open subset $U$ of $A$ containing $a$, we can consider taking the derivative of $Df$ at some $a \in A$. If $(Df)(a)$ exists for every $a \in A$, we get a mapping $D^2f: A \to \mathcal{L}(E; \mathcal{L}(E; F))$, where $D^2f(a) = D(Df)(a)$, for every $a \in A$. If $D^2f(a)$ exists, then for every $u \in E$,

$$D^2f(a)(u) = D(Df)(a)(u) = D_u(Df)(a) \in \mathcal{L}(E; F).$$

Recall from Proposition 19.19, that the map $app$ from $\mathcal{L}(E; F) \times E$ to $F$, defined such that for every $L \in \mathcal{L}(E; F)$, for every $v \in E$,

$$app(L, v) = L(v),$$

is a continuous bilinear map. Thus, in particular, given a fixed $v \in E$, the linear map $app_v: \mathcal{L}(E; F) \to F$, defined such that $app_v(L) = L(v)$, is a continuous map.

Also recall from Proposition 20.7, that if $h: A \to G$ is a function such that $Dh(a)$ exits, and $k: G \to H$ is a continuous linear map, then, $D(k \circ h)(a)$ exists, and

$$k(Dh(a)(u)) = D(k \circ h)(a)(u),$$

that is,

$$k(D_uf(a)) = D_u(k \circ h)(a),$$

Applying these two facts to $h = Df$, and to $k = app_v$, we have

$$D_u(Df)(a)(v) = D_u(app_v \circ Df)(a).$$

But $(app_v \circ Df)(x) = Df(x)(v) = D_v f(x)$, for every $x \in A$, that is, $app_v \circ Df = D_v f$ on $A$. So, we have

$$D_u(Df)(a)(v) = D_u(D_v f)(a),$$

and since $D^2f(a)(u) = D_u(Df)(a)$, we get

$$D^2f(a)(u)(v) = D_u(D_v f)(a).$$

Thus, when $D^2f(a)$ exists, $D_u(D_v f)(a)$ exists, and

$$D^2f(a)(u)(v) = D_u(D_v f)(a),$$

for all $u, v \in E$. We also denote $D_u(D_v f)(a)$ by $D^2_{u,v} f(a)$, or $D_uD_v f(a)$.

Recall from Proposition 19.18, that the map from $\mathcal{L}_2(E, E; F)$ to $\mathcal{L}(E; \mathcal{L}(E; F))$ defined such that $g \mapsto \varphi$ iff for every $g \in \mathcal{L}_2(E, E; F)$,

$$\varphi(u)(v) = g(u, v),$$
is an isomorphism of vector spaces. Thus, we will consider \( D^2 f(a) \in \mathcal{L}(E; \mathcal{L}(E; F)) \) as a continuous bilinear map in \( \mathcal{L}_2(E, E; F) \), and we will write \( D^2 f(a)(u, v) \), instead of \( D^2 f(a)(u)(v) \).

Then, the above discussion can be summarized by saying that when \( D^2 f(a) \) is defined, we have

\[
D^2 f(a)(u, v) = D_u D_v f(a).
\]

When \( E \) has finite dimension and \((e_1, \ldots, e_n)\) is a basis for \( E \), we denote \( D_{e_j} D_{e_i} f(a) \) by \( \frac{\partial^2 f}{\partial x_i \partial x_j}(a) \), when \( i \neq j \), and we denote \( D_{e_i} D_{e_i} f(a) \) by \( \frac{\partial^2 f}{\partial x_i^2}(a) \).

The following important lemma attributed to Schwarz can be shown, using Lemma 20.12. Given a bilinear map \( f: E \times E \rightarrow F \), recall that \( f \) is symmetric, if

\[
f(u, v) = f(v, u),
\]

for all \( u, v \in E \).

**Lemma 3.18.** (Schwarz’s lemma) Given two normed vector spaces \( E \) and \( F \), given any open subset \( A \) of \( E \), given any \( f: A \rightarrow F \), for every \( a \in A \), if \( D^2 f(a) \) exists, then \( D^2 f(a) \in \mathcal{L}_2(E, E; F) \) is a continuous symmetric bilinear map. As a corollary, if \( E \) is of finite dimension \( n \), and \((e_1, \ldots, e_n)\) is a basis for \( E \), we have

\[
\frac{\partial^2 f}{\partial x_i \partial x_j}(a) = \frac{\partial^2 f}{\partial x_j \partial x_i}(a).
\]

**Remark:** There is a variation of the above lemma which does not assume the existence of \( D^2 f(a) \), but instead assumes that \( D_u D_v f \) and \( D_v D_u f \) exist on an open subset containing \( a \) and are continuous at \( a \), and concludes that \( D_u D_v f(a) = D_v D_u f(a) \). This is just a different result which does not imply Lemma 20.18, and is not a consequence of Lemma 20.18.

When \( E = \mathbb{R}^2 \), the only existence of \( \frac{\partial^2 f}{\partial x \partial y}(a) \) and \( \frac{\partial^2 f}{\partial y \partial x}(a) \) is not sufficient to insure the existence of \( D^2 f(a) \).

When \( E \) if of finite dimension \( n \) and \((e_1, \ldots, e_n)\) is a basis for \( E \), if \( D^2 f(a) \) exists, for every \( u = u_1 e_1 + \cdots + u_n e_n \) and \( v = v_1 e_1 + \cdots + v_n e_n \) in \( E \), since \( D^2 f(a) \) is a symmetric bilinear form, we have

\[
D^2 f(a)(u, v) = \sum_{i=1, j=1}^{n} u_i v_j \frac{\partial^2 f}{\partial x_i \partial x_j}(a),
\]
which can be written in matrix form as:

\[
D^2 f(a)(u, v) = U^\top \begin{pmatrix}
\frac{\partial^2 f}{\partial x_1^2}(a) & \frac{\partial^2 f}{\partial x_1 \partial x_2}(a) & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n}(a) \\
\frac{\partial^2 f}{\partial x_1 \partial x_2}(a) & \frac{\partial^2 f}{\partial x_2^2}(a) & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_n}(a) \\
\vdots & \vdots & \ddots & \vdots \\
\frac{\partial^2 f}{\partial x_1 \partial x_n}(a) & \frac{\partial^2 f}{\partial x_2 \partial x_n}(a) & \cdots & \frac{\partial^2 f}{\partial x_n^2}(a)
\end{pmatrix} V
\]

where \( U \) is the column matrix representing \( u \), and \( V \) is the column matrix representing \( v \), over the basis \((e_1, \ldots, e_n)\).

The above symmetric matrix is called the Hessian of \( f \) at \( a \). If \( F \) itself is of finite dimension, and \((v_1, \ldots, v_m)\) is a basis for \( F \), then \( f = (f_1, \ldots, f_m) \), and each component \( D^2 f(a)_i(u, v) \) of \( D^2 f(a)(u, v) \) \((1 \leq i \leq m)\), can be written as

\[
D^2 f(a)_i(u, v) = U^\top \begin{pmatrix}
\frac{\partial^2 f_i}{\partial x_1^2}(a) & \frac{\partial^2 f_i}{\partial x_1 \partial x_2}(a) & \cdots & \frac{\partial^2 f_i}{\partial x_1 \partial x_n}(a) \\
\frac{\partial^2 f_i}{\partial x_1 \partial x_2}(a) & \frac{\partial^2 f_i}{\partial x_2^2}(a) & \cdots & \frac{\partial^2 f_i}{\partial x_2 \partial x_n}(a) \\
\vdots & \vdots & \ddots & \vdots \\
\frac{\partial^2 f_i}{\partial x_1 \partial x_n}(a) & \frac{\partial^2 f_i}{\partial x_2 \partial x_n}(a) & \cdots & \frac{\partial^2 f_i}{\partial x_n^2}(a)
\end{pmatrix} V
\]

Thus, we could describe the vector \( D^2 f(a)(u, v) \) in terms of an \( mn \times mn \)-matrix consisting of \( m \) diagonal blocks, which are the above Hessians, and the row matrix \((U^\top, \ldots, U^\top)\) \((m \text{ times})\) and the column matrix consisting of \( m \) copies of \( V \). In particular, if \( m = 1 \), that is, \( F = \mathbb{R} \) or \( F = \mathbb{C} \), then the Hessian matrix is an \( n \times n \) matrix.

We now indicate briefly how higher-order derivatives are defined. Let \( m \geq 2 \). Given a function \( f: A \to F \) as before, for any \( a \in A \), if the derivatives \( D^i f \) exist on \( A \) for all \( i, 1 \leq i \leq m - 1 \), by induction, \( D^{m-1} f \) can be considered to be a continuous function \( D^{m-1} f: A \to L_{m-1}(E^{m-1}; F) \), and we define

\[
D^m f(a) = D(D^{m-1} f)(a).
\]

Then, \( D^m f(a) \) can be identified with a continuous \( m \)-multilinear map in \( L_m(E^m; F) \). We can then show (as we did before), that if \( D^m f(a) \) is defined, then

\[
D^m f(a)(u_1, \ldots, u_m) = D_{u_1} \ldots D_{u_m} f(a).
\]

When \( E \) if of finite dimension \( n \) and \((e_1, \ldots, e_n)\) is a basis for \( E \), if \( D^m f(a) \) exists, for every \( j_1, \ldots, j_m \in \{1, \ldots, n\} \), we denote \( D e_{j_m} \ldots D e_{j_1} f(a) \) by

\[
\frac{\partial^m f}{\partial x_{j_1} \ldots \partial x_{j_m}}(a).
\]
Given a $m$-multilinear map $f \in \mathcal{L}_m(E^m; F)$, recall that $f$ is symmetric if
\[ f(u_{\pi(1)}, \ldots, u_{\pi(m)}) = f(u_1, \ldots, u_m), \]
for all $u_1, \ldots, u_m \in E$, and all permutations $\pi$ on $\{1, \ldots, m\}$. Then, the following generalization of Schwarz’s lemma holds.

**Lemma 3.19.** Given two normed vector spaces $E$ and $F$, given any open subset $A$ of $E$, given any $f: A \to F$, for every $a \in A$, for every $m \geq 1$, if $D^m f(a)$ exists, then $D^m f(a) \in \mathcal{L}_m(E^m; F)$ is a continuous symmetric $m$-multilinear map. As a corollary, if $E$ is of finite dimension $n$, and $(e_1, \ldots, e_n)$ is a basis for $E$, we have
\[ \frac{\partial^m f}{\partial x_{j_1} \cdots \partial x_{j_m}}(a) = \frac{\partial^m f}{\partial x_{\pi(j_1)} \cdots \partial x_{\pi(j_m)}}(a), \]
for every $j_1, \ldots, j_m \in \{1, \ldots, n\}$, and for every permutation $\pi$ on $\{1, \ldots, m\}$.

If $E$ is of finite dimension $n$, and $(e_1, \ldots, e_n)$ is a basis for $E$, $D^m f(a)$ is a symmetric $m$-multilinear map, and we have
\[ D^m f(a)(u_1, \ldots, u_m) = \sum_j u_{1,j_1} \cdots u_{m,j_m} \frac{\partial^m f}{\partial x_{j_1} \cdots \partial x_{j_m}}(a), \]
where $j$ ranges over all functions $j: \{1, \ldots, m\} \to \{1, \ldots, n\}$, for any $m$ vectors
\[ u_j = u_{j,1}e_1 + \cdots + u_{j,n}e_n. \]

The concept of $C^1$-function is generalized to the concept of $C^m$-function, and Theorem 20.13 can also be generalized.

**Definition 3.9.** Given two normed vector spaces $E$ and $F$, and an open subset $A$ of $E$, for any $m \geq 1$, we say that a function $f: A \to F$ is of class $C^m$ on $A$ or a $C^m$-function on $A$ if $D^k f$ exists and is continuous on $A$ for every $k$, $1 \leq k \leq m$. We say that $f: A \to F$ is of class $C^\infty$ on $A$ or a $C^\infty$-function on $A$ if $D^k f$ exists and is continuous on $A$ for every $k \geq 1$. A $C^\infty$-function (on $A$) is also called a smooth function (on $A$). A $C^m$-diffeomorphism $f: A \to B$ between $A$ and $B$ (where $A$ is an open subset of $E$ and $B$ is an open subset of $B$) is a bijection between $A$ and $B = f(A)$, such that both $f: A \to B$ and its inverse $f^{-1}: B \to A$ are $C^m$-functions.

Equivalently, $f$ is a $C^m$-function on $A$ if $f$ is a $C^1$-function on $A$ and $Df$ is a $C^{m-1}$-function on $A$.

We have the following theorem giving a necessary and sufficient condition for $f$ to be a $C^m$-function on $A$. A generalization to the case where $E = E_1 \oplus \cdots \oplus E_n$ also holds.
Theorem 3.20. Given two normed vector spaces $E$ and $F$, where $E$ is of finite dimension $n$, and where $(u_1, \ldots, u_n)$ is a basis of $E$, given any open subset $A$ of $E$, given any function $f: A \to F$, for any $m \geq 1$, the derivative $D^m f$ is a $C^m$-function on $A$ if and only if every partial derivative $D_{u_{j_k}} \ldots D_{u_{j_1}} f$ (or $\frac{\partial^k f}{\partial x_{j_k} \ldots \partial x_{j_1}}(a)$) is defined and continuous on $A$, for all $k$, $1 \leq k \leq m$, and all $j_1, \ldots, j_k \in \{1, \ldots, n\}$. As a corollary, if $F$ is of finite dimension $p$, and $(v_1, \ldots, v_p)$ is a basis of $F$, the derivative $D^m f$ is defined and continuous on $A$ if and only if every partial derivative $D_{u_{j_k}} \ldots D_{u_{j_1}} f_i$ (or $\frac{\partial^k f_i}{\partial x_{j_k} \ldots \partial x_{j_1}}(a)$) is defined and continuous on $A$, for all $i$, $1 \leq i \leq p$, and all $j_1, \ldots, j_k \in \{1, \ldots, n\}$.

When $E = \mathbb{R}$ (or $E = \mathbb{C}$), for any $a \in E$, $D^m f(a)(1, \ldots, 1)$ is a vector in $F$, called the $m$th-order vector derivative. As in the case $m = 1$, we will usually identify the multilinear map $D^m f(a)$ with the vector $D^m f(a)(1, \ldots, 1)$. Some notational conventions can also be introduced to simplify the notation of higher-order derivatives, and we discuss such conventions very briefly.

Recall that when $E$ is of finite dimension $n$, and $(e_1, \ldots, e_n)$ is a basis for $E$, $D^m f(a)$ is a symmetric $m$-multilinear map, and we have

$$D^m f(a)(u_1, \ldots, u_m) = \sum_j u_{1,j_1} \ldots u_{m,j_m} \frac{\partial^m f}{\partial x_{j_1} \ldots \partial x_{j_m}}(a),$$

where $j$ ranges over all functions $j: \{1, \ldots, m\} \to \{1, \ldots, n\}$, for any $m$ vectors

$$u_j = u_{j,1} e_1 + \cdots + u_{j,n} e_n.$$

We can then group the various occurrences of $\partial x_{j_k}$ corresponding to the same variable $x_{j_k}$, and this leads to the notation

$$\left(\frac{\partial}{\partial x_1}\right)^{\alpha_1} \left(\frac{\partial}{\partial x_2}\right)^{\alpha_2} \cdots \left(\frac{\partial}{\partial x_n}\right)^{\alpha_n} f(a),$$

where $\alpha_1 + \alpha_2 + \cdots + \alpha_m = m$.

If we denote $(\alpha_1, \ldots, \alpha_n)$ simply by $\alpha$, then we denote

$$\left(\frac{\partial}{\partial x_1}\right)^{\alpha_1} \left(\frac{\partial}{\partial x_2}\right)^{\alpha_2} \cdots \left(\frac{\partial}{\partial x_n}\right)^{\alpha_n} f$$

by

$$\partial^\alpha f,$$

or

$$\left(\frac{\partial}{\partial x}\right)^\alpha f.$$

If $\alpha = (\alpha_1, \ldots, \alpha_n)$, we let $|\alpha| = \alpha_1 + \alpha_2 + \cdots + \alpha_n$, $\alpha! = \alpha_1! \cdots \alpha_n!$, and if $h = (h_1, \ldots, h_n)$, we denote $h_1^{\alpha_1} \cdots h_n^{\alpha_n}$ by $h^\alpha$.

In the next section, we survey various versions of Taylor’s formula.
3.5 Taylor’s Formula, Faà di Bruno’s Formula

We discuss, without proofs, several versions of Taylor’s formula. The hypotheses required in each version become increasingly stronger. The first version can be viewed as a generalization of the notion of derivative. Given an \( m \)-linear map \( f : E^m \to F \), for any vector \( h \in E \), we abbreviate

\[ f(h, \ldots, h) \]

by \( f(h^m) \). The version of Taylor’s formula given next is sometimes referred to as the formula of Taylor–Young.

**Theorem 3.21. (Taylor–Young)** Given two normed vector spaces \( E \) and \( F \), for any open subset \( A \subseteq E \), for any function \( f : A \to F \), for any \( a \in A \), if \( D^k f \) exists in \( A \) for all \( k \), \( 1 \leq k \leq m - 1 \), and if \( D^m f(a) \) exists, then we have:

\[
f(a + h) = f(a) + \frac{1}{1!} D^1 f(a)(h) + \cdots + \frac{1}{m!} D^m f(a)(h^m) + \|h\|^m \epsilon(h),
\]

for any \( h \) such that \( a + h \in A \), and where \( \lim_{h \to 0, h \neq 0} \epsilon(h) = 0 \).

The above version of Taylor’s formula has applications to the study of relative maxima (or minima) of real-valued functions. It is also used to study the local properties of curves and surfaces.

The next version of Taylor’s formula can be viewed as a generalization of Lemma 20.12. It is sometimes called the Taylor formula with Lagrange remainder or generalized mean value theorem.

**Theorem 3.22. (Generalized mean value theorem)** Let \( E \) and \( F \) be two normed vector spaces, let \( A \) be an open subset of \( E \), and let \( f : A \to F \) be a function on \( A \). Given any \( a \in A \) and any \( h \neq 0 \) in \( E \), if the closed segment \( [a, a + h] \) is contained in \( A \), \( D^k f \) exists in \( A \) for all \( k \), \( 1 \leq k \leq m \), \( D^{m+1} f(x) \) exists at every point \( x \) of the open segment \( [a, a + h] \), and

\[
\max_{x \in (a, a + h)} \|D^{m+1} f(x)\| \leq M,
\]

for some \( M \geq 0 \), then

\[
\left\| f(a + h) - f(a) - \left( \frac{1}{1!} D^1 f(a)(h) + \cdots + \frac{1}{m!} D^m f(a)(h^m) \right) \right\| \leq M \frac{\|h\|^{m+1}}{(m + 1)!}.
\]

As a corollary, if \( L : E^{m+1} \to F \) is a continuous \((m + 1)\)-linear map, then

\[
\left\| f(a + h) - f(a) - \left( \frac{1}{1!} D^1 f(a)(h) + \cdots + \frac{1}{m!} D^m f(a)(h^m) + \sum_{k=0}^{m+1} \frac{L(h^{m+1})}{(m + 1)!} \right) \right\| \leq M \frac{\|h\|^{m+1}}{(m + 1)!},
\]

where \( M = \max_{x \in (a, a + h)} \|D^{m+1} f(x) - L\| \).
The above theorem is sometimes stated under the slightly stronger assumption that \( f \) is a \( C^m \)-function on \( A \). If \( f : A \to \mathbb{R} \) is a real-valued function, Theorem 20.22 can be refined a little bit. This version is often called the formula of Taylor–Maclaurin.

**Theorem 3.23.** (Taylor–Maclaurin) Let \( E \) be a normed vector space, let \( A \) be an open subset of \( E \), and let \( f : A \to \mathbb{R} \) be a real-valued function on \( A \). Given any \( a \in A \) and any \( h \neq 0 \) in \( E \), if the closed segment \([a, a + h]\) is contained in \( A \), if \( D^k f \) exists in \( A \) for all \( k \), \( 1 \leq k \leq m \), and \( D^{m+1} f(x) \) exists at every point \( x \) of the open segment \([a, a + h]\), then there is some \( \theta \in \mathbb{R} \), with \( 0 < \theta < 1 \), such that

\[
f(a + h) = f(a) + \frac{1}{1!} D^1 f(a)(h) + \cdots + \frac{1}{m!} D^m f(a)(h^m) + \frac{1}{(m+1)!} D^{m+1} f(a + \theta h)(h^{m+1}).
\]

We also mention for “mathematical culture,” a version with integral remainder, in the case of a real-valued function. This is usually called Taylor’s formula with integral remainder.

**Theorem 3.24.** (Taylor’s formula with integral remainder) Let \( E \) be a normed vector space, let \( A \) be an open subset of \( E \), and let \( f : A \to \mathbb{R} \) be a real-valued function on \( A \). Given any \( a \in A \) and any \( h \neq 0 \) in \( E \), if the closed segment \([a, a + h]\) is contained in \( A \), and if \( f \) is a \( C^{m+1} \)-function on \( A \), then we have

\[
f(a + h) = f(a) + \frac{1}{1!} D^1 f(a)(h) + \cdots + \frac{1}{m!} D^m f(a)(h^m) + \int_0^1 \frac{(1-t)^m}{m!} [D^{m+1} f(a + th)(h^{m+1})] dt.
\]

The advantage of the above formula is that it gives an explicit remainder. We now examine briefly the situation where \( E \) is of finite dimension \( n \), and \((e_1, \ldots, e_n)\) is a basis for \( E \). In this case, we get a more explicit expression for the expression

\[
\sum_{k=0}^{k=m} \frac{1}{k!} D^k f(a)(h^k)
\]

involved in all versions of Taylor’s formula, where by convention, \( D^0 f(a)(h^0) = f(a) \). If \( h = h_1 e_1 + \cdots + h_n e_n \), then we have

\[
\sum_{k=0}^{k=m} \frac{1}{k!} D^k f(a)(h^k) = \sum_{k_1 + \cdots + k_n \leq m} \frac{h_1^{k_1}}{k_1!} \cdots \frac{h_n^{k_n}}{k_n!} \left( \frac{\partial}{\partial x_1} \right)^{k_1} \cdots \left( \frac{\partial}{\partial x_n} \right)^{k_n} f(a),
\]

which, using the abbreviated notation introduced at the end of Section 20.4, can also be written as

\[
\sum_{k=0}^{k=m} \frac{1}{k!} D^k f(a)(h^k) = \sum_{|\alpha| \leq m} \frac{h^\alpha}{\alpha!} \partial^\alpha f(a).
\]
The advantage of the above notation is that it is the same as the notation used when \( n = 1 \), i.e., when \( E = \mathbb{R} \) (or \( E = \mathbb{C} \)). Indeed, in this case, the Taylor–Maclaurin formula reads as:

\[
f(a + h) = f(a) + \frac{h}{1!}D^1f(a) + \cdots + \frac{h^m}{m!}D^mf(a) + \frac{h^{m+1}}{(m+1)!}D^{m+1}f(a + \theta h),
\]

for some \( \theta \in \mathbb{R} \), with \( 0 < \theta < 1 \), where \( D^k f(a) \) is the value of the \( k \)-th derivative of \( f \) at \( a \) (and thus, as we have already said several times, this is the \( k \)th-order vector derivative, which is just a scalar, since \( F = \mathbb{R} \)).

In the above formula, the assumptions are that \( f: [a, a + h] \to \mathbb{R} \) is a \( C^m \)-function on \([a, a + h] \), and that \( D^{m+1}f(x) \) exists for every \( x \in (a, a + h) \).

Taylor’s formula is useful to study the local properties of curves and surfaces. In the case of a curve, we consider a function \( f: [r, s] \to F \) from a closed interval \([r, s] \) of \( \mathbb{R} \) to some vector space \( F \), the derivatives \( D^k f(a)(h^k) \) correspond to vectors \( h^k D^k f(a) \), where \( D^k f(a) \) is the \( k \)th vector derivative of \( f \) at \( a \) (which is really \( D^k f(a)(1, \ldots, 1) \)), and for any \( a \in (r, s) \), Theorem 20.21 yields the following formula:

\[
f(a + h) = f(a) + \frac{h}{1!}D^1f(a) + \cdots + \frac{h^m}{m!}D^mf(a) + h^m \epsilon(h),
\]

for any \( h \) such that \( a + h \in (r, s) \), and where \( \lim_{h \to 0, h \neq 0} \epsilon(h) = 0 \).

In the case of functions \( f: \mathbb{R}^n \to \mathbb{R} \), it is convenient to have formulae for the Taylor–Young formula and the Taylor–Maclaurin formula in terms of the gradient and the Hessian. Recall that the gradient \( \nabla f(a) \) of \( f \) at \( a \in \mathbb{R}^n \) is the column vector

\[
\nabla f(a) = \begin{pmatrix}
\frac{\partial f}{\partial x_1}(a) \\
\frac{\partial f}{\partial x_2}(a) \\
\vdots \\
\frac{\partial f}{\partial x_n}(a)
\end{pmatrix},
\]

and that

\[
f'(a)(u) = Df(a)(u) = \nabla f(a) \cdot u,
\]

for any \( u \in \mathbb{R}^n \) (where \( \cdot \) means inner product). The above equation shows that the direction of the gradient \( \nabla f(a) \) is the direction of maximal increase of the function \( f \) at \( a \) and that \( ||\nabla f(a)|| \) is the rate of change of \( f \) in its direction of maximal increase. This is the reason why methods of “gradient descent” pick the direction opposite to the gradient (we are trying to minimize \( f \)).
The Hessian matrix $\nabla^2 f(a)$ of $f$ at $a \in \mathbb{R}^n$ is the $n \times n$ symmetric matrix

$$\nabla^2 f(a) = \begin{pmatrix}
\frac{\partial^2 f}{\partial x_1^2}(a) & \frac{\partial^2 f}{\partial x_1 \partial x_2}(a) & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n}(a) \\
\frac{\partial^2 f}{\partial x_2 \partial x_1}(a) & \frac{\partial^2 f}{\partial x_2^2}(a) & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_n}(a) \\
\vdots & \vdots & \ddots & \vdots \\
\frac{\partial^2 f}{\partial x_n \partial x_1}(a) & \frac{\partial^2 f}{\partial x_n \partial x_2}(a) & \cdots & \frac{\partial^2 f}{\partial x_n^2}(a)
\end{pmatrix},$$

and we have

$$D^2 f(a)(u, v) = u^\top \nabla^2 f(a)v = u \cdot \nabla^2 f(a)v = \nabla^2 f(a)u \cdot v,$$

for all $u, v \in \mathbb{R}^n$. Then, we have the following three formulations of the formula of Taylor–Young of order 2:

$$f(a + h) = f(a) + Df(a)(h) + \frac{1}{2}D^2 f(a)(h, h) + \|h\|^2 \epsilon(h)$$
$$f(a + h) = f(a) + \nabla f(a) \cdot h + \frac{1}{2}(h \cdot \nabla^2 f(a)h) + (h \cdot h)\epsilon(h)$$
$$f(a + h) = f(a) + (\nabla f(a))^\top h + \frac{1}{2}(h^\top \nabla^2 f(a)h) + (h^\top h)\epsilon(h),$$

with $\lim_{h \to 0} \epsilon(h) = 0$.

One should keep in mind that only the first formula is intrinsic (i.e., does not depend on the choice of a basis), whereas the other two depend on the basis and the inner product chosen on $\mathbb{R}^n$. As an exercise, the reader should write similar formulae for the Taylor–Maclaurin formula of order 2.

Another application of Taylor’s formula is the derivation of a formula which gives the $m$th derivative of the composition of two functions, usually known as “Faà di Bruno’s formula.” This formula is useful when dealing with geometric continuity of splines curves and surfaces.

**Proposition 3.25.** Given any normed vector space $E$, for any function $f : \mathbb{R} \to \mathbb{R}$ and any function $g : \mathbb{R} \to E$, for any $a \in \mathbb{R}$, letting $b = f(a)$, $f^{(i)}(a) = D^i f(a), \text{ and } g^{(i)}(b) = D^i g(b)$, for any $m \geq 1$, if $f^{(i)}(a)$ and $g^{(i)}(b)$ exist for all $i, 1 \leq i \leq m$, then $(g \circ f)^{(m)}(a) = D^m (g \circ f)(a)$ exists and is given by the following formula:

$$(g \circ f)^{(m)}(a) = \sum_{0 \leq j \leq m} \sum_{\sum_{i_1, i_2, \ldots, i_m = j} i_1 + i_2 + \cdots + i_m} \frac{m!}{i_1! \cdots i_m!} g^{(j)}(b) \left( \frac{f^{(1)}(a)}{1!} \right)^{i_1} \cdots \left( \frac{f^{(m)}(a)}{m!} \right)^{i_m}.$$

When $m = 1$, the above simplifies to the familiar formula

$$(g \circ f)'(a) = g'(b)f'(a),$$

and for $m = 2$, we have

$$(g \circ f)^{(2)}(a) = g^{(2)}(b)(f^{(1)}(a))^2 + g^{(1)}(b)f^{(2)}(a).$$
3.6 Further Readings

A thorough treatment of differential calculus can be found in Munkres [77], Lang [66], Schwartz [92], Cartan [26], and Avez [7]. The techniques of differential calculus have many applications, especially to the geometry of curves and surfaces and to differential geometry in general. For this, we recommend do Carmo [36, 37] (two beautiful classics on the subject), Kreyszig [62], Stoker [100], Gray [50], Berger and Gostiaux [11], Milnor [76], Lang [64], Warner [112] and Choquet-Bruhat [28].

3.7 Summary

The main concepts and results of this chapter are listed below:

- **Directional derivative** ($D_{\alpha} f(a)$).
- **Total derivative, Fréchet derivative, derivative, total differential, differential** ($df(a), df$).
- **Partial derivatives**.
- **Affine functions**.
- **The chain rule**.
- **Jacobian matrices** ($J(f)(a)$) **Jacobians**.
- **Gradient of a function** ($\text{grad} f(a), \nabla f(a)$).
- **Mean value theorem**.
- **$C^0$-functions, $C^1$-functions**.
- **The implicit function theorem**.
- **Local homeomorphisms, local diffeomorphisms, diffeomorphisms**.
- **The inverse function theorem**.
- **Immersions, submersions**.
- **Second-order derivatives**.
- **Schwarz’s lemma**.
- **Hessian matrix**.
- **$C^\infty$-functions, smooth functions**.
• Taylor–Young’s formula.
• Generalized mean value theorem.
• Taylor–MacLaurin’s formula.
• Taylor’s formula with integral remainder.
• Faà di Bruno’s formula.
Chapter 4

Extrema of Real-Valued Functions

4.1 Local Extrema, Constrained Local Extrema, and Lagrange Multipliers

Let $J: E \to \mathbb{R}$ be a real-valued function defined on a normed vector space $E$ (or more generally, any topological space). Ideally we would like to find where the function $J$ reaches a minimum or a maximum value, at least locally. In this chapter we will usually use the notations $dJ(u)$ or $J'(u)$ (or $dJ_u$ or $J'_u$) for the derivative of $J$ at $u$, instead of $DJ(u)$. Our presentation follows very closely that of Ciarlet [30] (Chapter 7), which we find to be one of the clearest.

**Definition 4.1.** If $J: E \to \mathbb{R}$ is a real-valued function defined on a normed vector space $E$, we say that $J$ has a local minimum (or relative minimum) at the point $u \in E$ if there is some open subset $W \subseteq E$ containing $u$ such that

$$J(u) \leq J(w) \quad \text{for all } w \in W.$$ 

Similarly, we say that $J$ has a local maximum (or relative maximum) at the point $u \in E$ if there is some open subset $W \subseteq E$ containing $u$ such that

$$J(u) \geq J(w) \quad \text{for all } w \in W.$$ 

In either case, we say that $J$ has a local extremum (or relative extremum) at $u$. We say that $J$ has a strict local minimum (resp. strict local maximum) at the point $u \in E$ if there is some open subset $W \subseteq E$ containing $u$ such that

$$J(u) < J(w) \quad \text{for all } w \in W - \{u\}$$

(resp. 

$$J(u) > J(w) \quad \text{for all } w \in W - \{u\}).$$
By abuse of language, we often say that the point \( u \) itself “is a local minimum” or a “local maximum,” even though, strictly speaking, this does not make sense.

We begin with a well-known necessary condition for a local extremum.

**Proposition 4.1.** Let \( E \) be a normed vector space and let \( J : \Omega \to \mathbb{R} \) be a function, with \( \Omega \) some open subset of \( E \). If the function \( J \) has a local extremum at some point \( u \in \Omega \) and if \( J \) is differentiable at \( u \), then

\[
dJ_u = J'(u) = 0.
\]

*Proof.* Pick any \( v \in E \). Since \( \Omega \) is open, for \( t \) small enough we have \( u + tv \in \Omega \), so there is an open interval \( I \subseteq \mathbb{R} \) such that the function \( \varphi \) given by

\[
\varphi(t) = J(u + tv)
\]

for all \( t \in I \) is well-defined. By applying the chain rule, we see that \( \varphi \) is differentiable at \( t = 0 \), and we get

\[
\varphi'(0) = dJ_u(v).
\]

Without loss of generality, assume that \( u \) is a local minimum. Then we have

\[
\varphi'(0) = \lim_{t \to 0^-} \frac{\varphi(t) - \varphi(0)}{t} \leq 0
\]

and

\[
\varphi'(0) = \lim_{t \to 0^+} \frac{\varphi(t) - \varphi(0)}{t} \geq 0,
\]

which shows that \( \varphi'(0) = dJ_u(v) = 0 \). As \( v \in E \) is arbitrary, we conclude that \( dJ_u = 0 \). \( \square \)

A point \( u \in \Omega \) such that \( J'(u) = 0 \) is called a critical point of \( J \).

If \( E = \mathbb{R}^n \), then the condition \( dJ_u = 0 \) is equivalent to the system

\[
\frac{\partial J}{\partial x_1}(u_1, \ldots, u_n) = 0,
\]

\[
\vdots
\]

\[
\frac{\partial J}{\partial x_n}(u_1, \ldots, u_n) = 0.
\]

The condition of Proposition 21.1 is only a necessary condition for the existence of an extremum, but not a sufficient condition. Here are some counter-examples. If \( f : \mathbb{R} \to \mathbb{R} \) is the function given by \( f(x) = x^3 \), since \( f'(x) = 3x^2 \), we have \( f'(0) = 0 \), but 0 is neither a minimum nor a maximum of \( f \). If \( g : \mathbb{R}^2 \to \mathbb{R} \) is the function given by \( g(x, y) = x^2 - y^2 \), then \( g'_{(x,y)} = (2x - 2y) \), so \( g'_{(0,0)} = (0 0) \), yet near \((0,0)\) the function \( g \) takes negative and positive values.
In many practical situations, we need to look for local extrema of a function $J$ under additional constraints. This situation can be formalized conveniently as follows: We have a function $J: \Omega \rightarrow \mathbb{R}$ defined on some open subset $\Omega$ of a normed vector space, but we also have some subset $U$ of $\Omega$, and we are looking for the local extrema of $J$ with respect to the set $U$.

The elements $u \in U$ are often called feasible solutions of the optimization problem consisting in finding the local extrema of some objective function $J$ with respect to some subset $U$ of $\Omega$ defined by a set of constraints. Note that in most cases, $U$ is not open. In fact, $U$ is usually closed.

**Definition 4.2.** If $J: \Omega \rightarrow \mathbb{R}$ is a real-valued function defined on some open subset $\Omega$ of a normed vector space $E$ and if $U$ is some subset of $\Omega$, we say that $J$ has a local minimum (or relative minimum) at the point $u \in U$ with respect to $U$ if there is some open subset $W \subseteq \Omega$ containing $u$ such that

$$J(u) \leq J(w) \quad \text{for all } w \in U \cap W.$$  

Similarly, we say that $J$ has a local maximum (or relative maximum) at the point $u \in U$ with respect to $U$ if there is some open subset $W \subseteq \Omega$ containing $u$ such that

$$J(u) \geq J(w) \quad \text{for all } w \in U \cap W.$$  

In either case, we say that $J$ has a local extremum at $u$ with respect to $U$.

It is very important to note that the hypothesis that $\Omega$ is open is crucial for the validity of Proposition 21.1. For example, if $J$ is the identity function on $\mathbb{R}$ and $U = [0, 1]$, a closed subset, then $J'(x) = 1$ for all $x \in [0, 1]$, even though $J$ has a minimum at $x = 0$ and a maximum at $x = 1$.

Therefore, in order to find necessary conditions for a function $J: \Omega \rightarrow \mathbb{R}$ to have a local extremum with respect to a subset $U$ of $\Omega$ (where $\Omega$ is open), we need to somehow incorporate the definition of $U$ into these conditions. This can be done in two cases:

1. The set $U$ is defined by a set of equations,

$$U = \{x \in \Omega \mid \varphi_i(x) = 0, \ 1 \leq i \leq m\},$$

where the functions $\varphi_i: \Omega \rightarrow \mathbb{R}$ are continuous (and usually differentiable).

2. The set $U$ is defined by a set of inequalities,

$$U = \{x \in \Omega \mid \varphi_i(x) \leq 0, \ 1 \leq i \leq m\},$$

where the functions $\varphi_i: \Omega \rightarrow \mathbb{R}$ are continuous (and usually differentiable).
In (1), the equations \( \varphi_i(x) = 0 \) are called equality constraints, and in (2), the inequalities \( \varphi_i(x) \leq 0 \) are called inequality constraints.

An inequality constraint of the form \( \varphi_i(x) \geq 0 \) is equivalent to the inequality constraint \( -\varphi_i(x) \leq 0 \). An equality constraint \( \varphi_i(x) = 0 \) is equivalent to the conjunction of the two inequality constraints \( \varphi_i(x) \leq 0 \) and \( -\varphi_i(x) \leq 0 \), so the case of inequality constraints subsumes the case of equality constraints. However, the case of equality constraints is easier to deal with, and in this chapter we will restrict our attention to this case.

If the functions \( \varphi_i \) are convex and \( \Omega \) is convex, then \( U \) is convex. This is a very important case that we will discuss later. In particular, if the functions \( \varphi_i \) are affine, then the equality constraints can be written as \( Ax = b \), and the inequality constraints as \( Ax \leq b \), for some \( m \times n \) matrix \( A \) and some vector \( b \in \mathbb{R}^m \). We will also discuss the case of affine constraints later.

In the case of equality constraints, a necessary condition for a local extremum with respect to \( U \) can be given in terms of Lagrange multipliers. In the case of inequality constraints, there is also a necessary condition for a local extremum with respect to \( U \) in terms of generalized Lagrange multipliers and the Karush–Kuhn–Tucker conditions. This will be discussed in Chapter 31.

We begin by considering the case where \( \Omega \subseteq E_1 \times E_2 \) is an open subset of a product of normed vector spaces and where \( U \) is the zero locus of some continuous function \( \varphi: \Omega \to E_2 \), which means that

\[
U = \{(u_1, u_2) \in \Omega \mid \varphi(u_1, u_2) = 0\}.
\]

For the sake of brevity, we say that \( J \) has a constrained local extremum at \( u \) instead of saying that \( J \) has a local extremum at the point \( u \in U \) with respect to \( U \). Fortunately, there is a necessary condition for constrained local extrema in terms of Lagrange multipliers.

**Theorem 4.2.** (Necessary condition for a constrained extremum) Let \( \Omega \subseteq E_1 \times E_2 \) be an open subset of a product of normed vector spaces, with \( E_1 \) a Banach space (\( E_1 \) is complete), let \( \varphi: \Omega \to E_2 \) be a \( C^1 \)-function (which means that \( d\varphi(\omega) \) exists and is continuous for all \( \omega \in \Omega \)), and let

\[
U = \{(u_1, u_2) \in \Omega \mid \varphi(u_1, u_2) = 0\}.
\]

Moreover, let \( u = (u_1, u_2) \in U \) be a point such that

\[
\frac{\partial \varphi}{\partial x_2}(u_1, u_2) \in \mathcal{L}(E_2; E_2) \quad \text{and} \quad \left( \frac{\partial \varphi}{\partial x_2}(u_1, u_2) \right)^{-1} \in \mathcal{L}(E_2; E_2),
\]

and let \( J: \Omega \to \mathbb{R} \) be a function which is differentiable at \( u \). If \( J \) has a constrained local extremum at \( u \), then there is a continuous linear form \( \Lambda(u) \in \mathcal{L}(E_2; \mathbb{R}) \) such that

\[
dJ(u) + \Lambda(u) \circ d\varphi(u) = 0.
\]
4.1. LOCAL EXTREMA AND LAGRANGE MULTIPLIERS

Proof. The plan of attack is to use the implicit function theorem; Theorem 20.14. Observe that the assumptions of Theorem 20.14 are indeed met. Therefore, there exist some open subsets $U_1 \subseteq E_1, U_2 \subseteq E_2$, and a continuous function $g: U_1 \rightarrow U_2$ with $(u_1, u_2) \in U_1 \times U_2 \subseteq \Omega$ and such that

$$\varphi(v_1, g(v_1)) = 0$$

for all $v_1 \in U_1$. Moreover, $g$ is differentiable at $u_1 \in U_1$ and

$$dg(u_1) = -\left( \frac{\partial \varphi}{\partial x_2}(u) \right)^{-1} \circ \frac{\partial \varphi}{\partial x_1}(u).$$

It follows that the restriction of $J$ to $(U_1 \times U_2) \cap U$ yields a function $G$ of a single variable, with

$$G(v_1) = J(v_1, g(v_1))$$

for all $v_1 \in U_1$. Now, the function $G$ is differentiable at $u_1$ and it has a local extremum at $u_1$ on $U_1$, so Proposition 21.1 implies that

$$dG(u_1) = 0.$$

By the chain rule,

$$dG(u_1) = \frac{\partial J}{\partial x_1}(u) + \frac{\partial J}{\partial x_2}(u) \circ dg(u_1)$$

$$= \frac{\partial J}{\partial x_1}(u) - \frac{\partial J}{\partial x_2}(u) \circ \left( \frac{\partial \varphi}{\partial x_2}(u) \right)^{-1} \circ \frac{\partial \varphi}{\partial x_1}(u).$$

From $dG(u_1) = 0$, we deduce

$$\frac{\partial J}{\partial x_1}(u) = \frac{\partial J}{\partial x_2}(u) \circ \left( \frac{\partial \varphi}{\partial x_2}(u) \right)^{-1} \circ \frac{\partial \varphi}{\partial x_1}(u),$$

and since we also have

$$\frac{\partial J}{\partial x_2}(u) = \frac{\partial J}{\partial x_2}(u) \circ \left( \frac{\partial \varphi}{\partial x_2}(u) \right)^{-1} \circ \frac{\partial \varphi}{\partial x_2}(u),$$

if we let

$$\Lambda(u) = -\frac{\partial J}{\partial x_2}(u) \circ \left( \frac{\partial \varphi}{\partial x_2}(u) \right)^{-1},$$

then we get

$$dJ(u) = \frac{\partial J}{\partial x_1}(u) + \frac{\partial J}{\partial x_2}(u)$$

$$= \frac{\partial J}{\partial x_2}(u) \circ \left( \frac{\partial \varphi}{\partial x_2}(u) \right)^{-1} \circ \left( \frac{\partial \varphi}{\partial x_1}(u) + \frac{\partial \varphi}{\partial x_2}(u) \right)$$

$$= -\Lambda(u) \circ d\varphi(u),$$

which yields $dJ(u) + \Lambda(u) \circ d\varphi(u) = 0$, as claimed. \qed
In most applications, we have $E_1 = \mathbb{R}^{n-m}$ and $E_2 = \mathbb{R}^m$ for some integers $m, n$ such that $1 \leq m < n$, $\Omega$ is an open subset of $\mathbb{R}^n$, $J: \Omega \to \mathbb{R}$, and we have $m$ functions $\varphi_i: \Omega \to \mathbb{R}$ defining the subset

$$U = \{v \in \Omega \mid \varphi_i(v) = 0, \ 1 \leq i \leq m\}.$$  

Theorem 21.2 yields the following necessary condition:

**Theorem 4.3.** (Necessary condition for a constrained extremum in terms of Lagrange multipliers) Let $\Omega$ be an open subset of $\mathbb{R}^n$, consider $m$ $C^1$-functions $\varphi_i: \Omega \to \mathbb{R}$ (with $1 \leq m < n$), let

$$U = \{v \in \Omega \mid \varphi_i(v) = 0, \ 1 \leq i \leq m\},$$  

and let $u \in U$ be a point such that the derivatives $d\varphi_i(u) \in L(\mathbb{R}^n; \mathbb{R})$ are linearly independent; equivalently, assume that the $m \times n$ matrix $((\partial \varphi_i/\partial x_j)(u))$ has rank $m$. If $J: \Omega \to \mathbb{R}$ is a function which is differentiable at $u \in U$ and if $J$ has a local constrained extremum at $u$, then there exist $m$ numbers $\lambda_i(u) \in \mathbb{R}$, uniquely defined, such that

$$dJ(u) + \lambda_1(u)d\varphi_1(u) + \cdots + \lambda_m(u)d\varphi_m(u) = 0;$$

equivalently,

$$\nabla J(u) + \lambda_1(u)\nabla \varphi_1(u) + \cdots + \lambda_1(u)\nabla \varphi_m(u) = 0.$$  

**Proof.** The linear independence of the $m$ linear forms $d\varphi_i(u)$ is equivalent to the fact that the $m \times n$ matrix $A = ((\partial \varphi_i/\partial x_j)(u))$ has rank $m$. By reordering the columns, we may assume that the first $m$ columns are linearly independent. If we let $\varphi: \Omega \to \mathbb{R}^m$ be the function defined by

$$\varphi(v) = (\varphi_1(v), \ldots, \varphi_m(v))$$

for all $v \in \Omega$, then we see that $\partial \varphi/\partial x_2(u)$ is invertible and both $\partial \varphi/\partial x_2(u)$ and its inverse are continuous, so that Theorem 21.2 applies, and there is some (continuous) linear form $\Lambda(u) \in L(\mathbb{R}^m; \mathbb{R})$ such that

$$dJ(u) + \Lambda(u) \circ d\varphi(u) = 0.$$  

However, $\Lambda(u)$ is defined by some $m$-tuple $(\lambda_1(u), \ldots, \lambda_m(u)) \in \mathbb{R}^m$, and in view of the definition of $\varphi$, the above equation is equivalent to

$$dJ(u) + \lambda_1(u)d\varphi_1(u) + \cdots + \lambda_m(u)d\varphi_m(u) = 0.$$  

The uniqueness of the $\lambda_i(u)$ is a consequence of the linear independence of the $d\varphi_i(u)$.

The numbers $\lambda_i(u)$ involved in Theorem 21.3 are called the Lagrange multipliers associated with the constrained extremum $u$ (again, with some minor abuse of language). The linear independence of the linear forms $d\varphi_i(u)$ is equivalent to the fact that the Jacobian matrix $((\partial \varphi_i/\partial x_j)(u))$ of $\varphi = (\varphi_1, \ldots, \varphi_m)$ at $u$ has rank $m$. If $m = 1$, the linear independence of the $d\varphi_i(u)$ reduces to the condition $\nabla \varphi_1(u) \neq 0$.  


A fruitful way to reformulate the use of Lagrange multipliers is to introduce the notion of the Lagrangian associated with our constrained extremum problem. This is the function \( L: \Omega \times \mathbb{R}^m \to \mathbb{R} \) given by
\[
L(v, \lambda) = J(v) + \lambda_1 \varphi_1(v) + \cdots + \lambda_m \varphi_m(v),
\]
with \( \lambda = (\lambda_1, \ldots, \lambda_m) \). Then, observe that there exists some \( \mu = (\mu_1, \ldots, \mu_m) \) and some \( u \in U \) such that
\[
dJ(u) + \mu_1 d\varphi_1(u) + \cdots + \mu_m d\varphi_m(u) = 0
\]
if and only if
\[
dL(u, \mu) = 0,
\]
or equivalently
\[
\nabla L(u, \mu) = 0;
\]
that is, iff \((u, \lambda)\) is a critical point of the Lagrangian \( L \).

Indeed \( dL(u, \mu) = 0 \) if equivalent to
\[
\frac{\partial L}{\partial v}(u, \mu) = 0
\]
\[
\frac{\partial L}{\partial \lambda_1}(u, \mu) = 0
\]
\[
\vdots
\]
\[
\frac{\partial L}{\partial \lambda_m}(u, \mu) = 0,
\]
and since
\[
\frac{\partial L}{\partial v}(u, \mu) = dJ(u) + \mu_1 d\varphi_1(u) + \cdots + \mu_m d\varphi_m(u)
\]
and
\[
\frac{\partial L}{\partial \lambda_i}(u, \mu) = \varphi_i(u),
\]
we get
\[
dJ(u) + \mu_1 d\varphi_1(u) + \cdots + \mu_m d\varphi_m(u) = 0
\]
and
\[
\varphi_1(u) = \cdots = \varphi_m(u) = 0,
\]
that is, \( u \in U \).

If we write out explicitly the condition
\[
dJ(u) + \mu_1 d\varphi_1(u) + \cdots + \mu_m d\varphi_m(u) = 0,
\]
we get the \( n \times m \) system

\[
\frac{\partial J}{\partial x_1}(u) + \lambda_1 \frac{\partial \varphi_1}{\partial x_1}(u) + \cdots + \lambda_m \frac{\partial \varphi_m}{\partial x_1}(u) = 0 \\
\vdots \\
\frac{\partial J}{\partial x_n}(u) + \lambda_1 \frac{\partial \varphi_1}{\partial x_n}(u) + \cdots + \lambda_m \frac{\partial \varphi_m}{\partial x_n}(u) = 0,
\]

and it is important to note that the matrix of this system is the transpose of the Jacobian matrix of \( \varphi \) at \( u \). If we write \( \text{Jac}(J)(u) = (\partial \varphi_i/\partial x_j)(u) \) for the Jacobian matrix of \( J \) (at \( u \)), then the above system is written in matrix form as

\[
\nabla J(u) + (\text{Jac}(J)(u))^\top \lambda = 0,
\]

where \( \lambda \) is viewed as a column vector, and the Lagrangian is equal to

\[
L(u, \lambda) = J(u) + (\varphi_1(u), \ldots, \varphi_m(u))\lambda.
\]

**Remark:** If the Jacobian matrix \( \text{Jac}(J)(v) = ((\partial \varphi_i/\partial x_j)(v)) \) has rank \( m \) for all \( v \in U \) (which is equivalent to the linear independence of the linear forms \( d\varphi_i(v) \)), then we say that \( 0 \in \mathbb{R}^m \) is a regular value of \( \varphi \). In this case, it is known that

\[
U = \{ v \in \Omega \mid \varphi(v) = 0 \}
\]

is a smooth submanifold of dimension \( n - m \) of \( \mathbb{R}^n \). Furthermore, the set

\[
T_vU = \{ w \in \mathbb{R}^n \mid d\varphi_i(v)(w) = 0, \ 1 \leq i \leq m \} = \bigcap_{i=1}^m \text{Ker} \ d\varphi_i(v)
\]

is the tangent space to \( U \) at \( v \) (a vector space of dimension \( n - m \)). Then, the condition

\[
dJ(v) + \mu_1 d\varphi_1(v) + \cdots + \mu_m d\varphi_m(v) = 0
\]

implies that \( dJ(v) \) vanishes on the tangent space \( T_vU \). Conversely, if \( dJ(v)(w) = 0 \) for all \( w \in T_vU \), this means that \( dJ(v) \) is orthogonal (in the sense of Definition 9.3) to \( T_vU \). Since (by Theorem 9.1 (b)) the orthogonal of \( T_vU \) is the space of linear forms spanned by \( d\varphi_1(v), \ldots, d\varphi_m(v) \), it follows that \( dJ(v) \) must be a linear combination of the \( d\varphi_i(v) \). Therefore, when \( 0 \) is a regular value of \( \varphi \), Theorem 21.3 asserts that if \( u \in U \) is a local extremum of \( J \), then \( dJ(u) \) must vanish on the tangent space \( T_uU \). We can say even more. The subset \( Z(J) \) of \( \Omega \) given by

\[
Z(J) = \{ v \in \Omega \mid J(v) = J(u) \}
\]
4.1. LOCAL EXTREMA AND LAGRANGE MULTIPLIERS

(the level set of level $J(u)$) is a hypersurface in $\Omega$, and if $dJ(u) \neq 0$, the zero locus of $dJ(u)$ is the tangent space $T_uZ(J)$ to $Z(J)$ at $u$ (a vector space of dimension $n - 1$), where

$$T_uZ(J) = \{ w \in \mathbb{R}^n \mid dJ(u)(w) = 0 \}.$$ 

Consequently, Theorem 21.3 asserts that

$$T_uU \subseteq T_uZ(J);$$

this is a geometric condition.

The beauty of the Lagrangian is that the constraints $\{ \varphi_i(v) = 0 \}$ have been incorporated into the function $L(v, \lambda)$, and that the necessary condition for the existence of a constrained local extremum of $J$ is reduced to the necessary condition for the existence of a local extremum of the unconstrained $L$.

However, one should be careful to check that the assumptions of Theorem 21.3 are satisfied (in particular, the linear independence of the linear forms $d\varphi_i$). For example, let $J: \mathbb{R}^3 \to \mathbb{R}$ be given by

$$J(x, y, z) = x + y + z^2$$

and $g: \mathbb{R}^3 \to \mathbb{R}$ by

$$g(x, y, z) = x^2 + y^2.$$ 

Since $g(x, y, z) = 0$ iff $x = y = 0$, we have $U = \{(0, 0, z) \mid z \in \mathbb{R}\}$ and the restriction of $J$ to $U$ is given by

$$J(0, 0, z) = z^2,$$

which has a minimum for $z = 0$. However, a “blind” use of Lagrange multipliers would require that there is some $\lambda$ so that

$$\frac{\partial J}{\partial x}(0, 0, z) = \lambda \frac{\partial g}{\partial x}(0, 0, z), \quad \frac{\partial J}{\partial y}(0, 0, z) = \lambda \frac{\partial g}{\partial y}(0, 0, z), \quad \frac{\partial J}{\partial z}(0, 0, z) = \lambda \frac{\partial g}{\partial z}(0, 0, z),$$

and since

$$\frac{\partial g}{\partial x}(x, y, z) = 2x, \quad \frac{\partial g}{\partial y}(x, y, z) = 2y, \quad \frac{\partial g}{\partial z}(0, 0, z) = 0,$$

the partial derivatives above all vanish for $x = y = 0$, so at a local extremum we should also have

$$\frac{\partial J}{\partial x}(0, 0, z) = 0, \quad \frac{\partial J}{\partial y}(0, 0, z) = 0, \quad \frac{\partial J}{\partial z}(0, 0, z) = 0,$$

but this is absurd since

$$\frac{\partial J}{\partial x}(x, y, z) = 1, \quad \frac{\partial J}{\partial y}(x, y, z) = 1, \quad \frac{\partial J}{\partial z}(x, y, z) = 2z.$$

The reader should enjoy finding the reason for the flaw in the argument.
One should also keep in mind that Theorem 21.3 gives only a necessary condition. The \((u, \lambda)\) may not correspond to local extrema! Thus, it is always necessary to analyze the local behavior of \(J\) near a critical point \(u\). This is generally difficult, but in the case where \(J\) is affine or quadratic and the constraints are affine or quadratic, this is possible (although not always easy).

Let us apply the above method to the following example in which \(E_1 = \mathbb{R}, E_2 = \mathbb{R}, \Omega = \mathbb{R}^2,\) and

\[
J(x_1, x_2) = -x_2 \\
\varphi(x_1, x_2) = x_1^2 + x_2^2 - 1.
\]

Observe that

\[
U = \{(x_1, x_2) \in \mathbb{R}^2 \mid x_1^2 + x_2^2 = 1\}
\]

is the unit circle, and since

\[
\nabla \varphi(x_1, x_2) = \begin{pmatrix} 2x_1 \\ 2x_2 \end{pmatrix},
\]

it is clear that \(\nabla \varphi(x_1, x_2) \neq 0\) for every point \((x_1, x_2)\) on the unit circle. If we form the Lagrangian

\[
L(x_1, x_2, \lambda) = -x_2 + \lambda(x_1^2 + x_2^2 - 1),
\]

Theorem 21.3 says that a necessary condition for \(J\) to have a constrained local extremum is that \(\nabla L(x_1, x_2, \lambda) = 0\), so the following equations must hold:

\[
2\lambda x_1 = 0 \\
-1 + 2\lambda x_2 = 0 \\
x_1^2 + x_2^2 = 1.
\]

The second equation implies that \(\lambda \neq 0\), and then the first yields \(x_1 = 0\), so the third yields \(x_2 = \pm 1\), and we get two solutions:

\[
\lambda = \frac{1}{2}, \quad (x_1, x_2) = (0, 1) \\
\lambda = -\frac{1}{2}, \quad (x_1', x_2') = (0, -1).
\]

We can check immediately that the first solution is a minimum and the second is a maximum. The reader should look for a geometric interpretation of this problem.

Let us now consider the case in which \(J\) is a quadratic function of the form

\[
J(v) = \frac{1}{2} v^\top A v - v^\top b,
\]

where \(A\) is an \(n \times n\) symmetric matrix, \(b \in \mathbb{R}^n\), and the constraints are given by a linear system of the form

\[
Cv = d,
\]
4.2 Using Second Derivatives to Find Extrema

where $C$ is an $m \times n$ matrix with $m < n$ and $d \in \mathbb{R}^m$. We also assume that $C$ has rank $m$. In this case, the function $\varphi$ is given by

$$\varphi(v) = (Cv - d)^\top,$$

because we view $\varphi(v)$ as a row vector (and $v$ as a column vector), and since

$$d\varphi(v)(w) = C^\top w,$$

the condition that the Jacobian matrix of $\varphi$ at $u$ have rank $m$ is satisfied. The Lagrangian of this problem is

$$L(v, \lambda) = \frac{1}{2}v^\top Av - v^\top b + (Cv - d)^\top \lambda = \frac{1}{2}v^\top Av - v^\top b + \lambda^\top (Cv - d),$$

where $\lambda$ is viewed as a column vector. Now, because $A$ is a symmetric matrix, it is easy to show that

$$\nabla L(v, \lambda) = \begin{pmatrix} Av - b + C^\top \lambda \\ Cv - d \end{pmatrix}.$$

Therefore, the necessary condition for constrained local extrema is

$$Av + C^\top \lambda = b$$
$$Cv = d,$$

which can be expressed in matrix form as

$$\begin{pmatrix} A & C^\top \\ C & 0 \end{pmatrix} \begin{pmatrix} v \\ \lambda \end{pmatrix} = \begin{pmatrix} b \\ d \end{pmatrix},$$

where the matrix of the system is a symmetric matrix. We should not be surprised to find the system of Section 23, except for some renaming of the matrices and vectors involved. As we know from Section 23.2, the function $J$ has a minimum iff $A$ is positive definite, so in general, if $A$ is only a symmetric matrix, the critical points of the Lagrangian do not correspond to extrema of $J$.

We now investigate conditions for the existence of extrema involving the second derivative of $J$.

4.2 Using Second Derivatives to Find Extrema

For the sake of brevity, we consider only the case of local minima; analogous results are obtained for local maxima (replace $J$ by $-J$, since $\max_u J(u) = -\min_u -J(u)$). We begin with a necessary condition for an unconstrained local minimum.
Proposition 4.4. Let $E$ be a normed vector space and let $J: \Omega \to \mathbb{R}$ be a function, with $\Omega$ some open subset of $E$. If the function $J$ is differentiable in $\Omega$, if $J$ has a second derivative $D^2J(u)$ at some point $u \in \Omega$, and if $J$ has a local minimum at $u$, then

$$D^2J(u)(w, w) \geq 0 \quad \text{for all } w \in E.$$

Proof. Pick any nonzero vector $w \in E$. Since $\Omega$ is open, for $t$ small enough, $u + tw \in \Omega$ and $J(u + tw) \geq J(u)$, so there is some open interval $I \subseteq \mathbb{R}$ such that $u + tw \in \Omega$ and $J(u + tw) \geq J(u)$ for all $t \in I$. Using the Taylor–Young formula and the fact that we must have $dJ(u) = 0$ since $J$ has a local minimum at $u$, we get

$$0 \leq J(u + tw) - J(u) = \frac{t^2}{2} D^2J(u)(w, w) + t^2 \|w\|^2 \epsilon(tw),$$

with $\lim_{t \to 0} \epsilon(tw) = 0$, which implies that

$$D^2J(u)(w, w) \geq 0.$$

Since the argument holds for all $w \in E$ (trivially if $w = 0$), the proposition is proved. \qed

One should be cautioned that there is no converse to the previous proposition. For example, the function $f: x \mapsto x^3$ has no local minimum at 0, yet $df(0) = 0$ and $D^2f(0)(u, v) = 0$.

Similarly, the reader should check that the function $f: \mathbb{R}^2 \to \mathbb{R}$ given by

$$f(x, y) = x^2 - 3y^3$$

has no local minimum at $(0, 0)$; yet $df(0, 0) = 0$ and $D^2f(0, 0)(u, v) = 2u^2 \geq 0$.

When $E = \mathbb{R}^n$, Proposition 21.4 says that a necessary condition for having a local minimum is that the Hessian $\nabla^2 J(u)$ be positive semidefinite (it is always symmetric).

We now give sufficient conditions for the existence of a local minimum.

Theorem 4.5. Let $E$ be a normed vector space, let $J: \Omega \to \mathbb{R}$ be a function with $\Omega$ some open subset of $E$, and assume that $J$ is differentiable in $\Omega$ and that $dJ(u) = 0$ at some point $u \in \Omega$. The following properties hold:

1. If $D^2J(u)$ exists and if there is some number $\alpha \in \mathbb{R}$ such that $\alpha > 0$ and

$$D^2J(u)(w, w) \geq \alpha \|w\|^2 \quad \text{for all } w \in E,$$

then $J$ has a strict local minimum at $u$. 
4.2. USING SECOND DERIVATIVES TO FIND EXTREMA

(2) If $D^2J(v)$ exists for all $v \in \Omega$ and if there is a ball $B \subseteq \Omega$ centered at $u$ such that

$$D^2J(v)(w, w) \geq 0 \quad \text{for all } v \in B \text{ and all } w \in E,$$

then $J$ has a local minimum at $u$.

Proof. (1) Using the formula of Taylor–Young, for every vector $w$ small enough, we can write

$$J(u + w) - J(u) = \frac{1}{2} D^2J(u)(w, w) + \|w\|^2 \epsilon(w) \geq \left(\frac{1}{2} \alpha + \epsilon(w)\right) \|w\|^2$$

with $\lim_{w \to 0} \epsilon(w) = 0$. Consequently if we pick $r > 0$ small enough that $|\epsilon(w)| < \alpha$ for all $w$ with $\|w\| < r$, then $J(u + w) > J(u)$ for all $u + w \in B$, where $B$ is the open ball of center $u$ and radius $r$. This proves that $J$ has a local strict minimum at $u$.

(2) The formula of Taylor–Maclaurin shows that for all $u + w \in B$, we have

$$J(u + w) = J(u) + \frac{1}{2} D^2J(v)(w, w) \geq J(u),$$

for some $v \in (u, w + w)$. \hfill \square

There are no converses of the two assertions of Theorem 21.5. However, there is a condition on $D^2J(u)$ that implies the condition of Part (1). Since this condition is easier to state when $E = \mathbb{R}^n$, we begin with this case.

Recall that a $n \times n$ symmetric matrix $A$ is positive definite if $x^T A x > 0$ for all $x \in \mathbb{R}^n - \{0\}$. In particular, $A$ must be invertible.

**Proposition 4.6.** For any symmetric matrix $A$, if $A$ is positive definite, then there is some $\alpha > 0$ such that

$$x^T A x \geq \alpha \|x\|^2 \quad \text{for all } x \in \mathbb{R}^n.$$

Proof. Pick any norm in $\mathbb{R}^n$ (recall that all norms on $\mathbb{R}^n$ are equivalent). Since the unit sphere $S^{n-1} = \{x \in \mathbb{R}^n \mid ||x|| = 1\}$ is compact and since the function $f(x) = x^T A x$ is never zero on $S^{n-1}$, the function $f$ has a minimum $\alpha > 0$ on $S^{n-1}$. Using the usual trick that $x = \|x\|(x/\|x\|)$ for every nonzero vector $x \in \mathbb{R}^n$ and the fact that the inequality of the proposition is trivial for $x = 0$, from

$$x^T A x \geq \alpha \quad \text{for all } x \text{ with } \|x\| = 1,$$

we get

$$x^T A x \geq \alpha \|x\|^2 \quad \text{for all } x \in \mathbb{R}^n,$$

as claimed. \hfill \square
We can combine Theorem 21.5 and Proposition 21.6 to obtain a useful sufficient condition for the existence of a strict local minimum. First let us introduce some terminology.

**Definition 4.3.** Given a function \( J: \Omega \to \mathbb{R} \) as before, say that a point \( u \in \Omega \) is a nondegenerate critical point if \( dJ(u) = 0 \) and if the Hessian matrix \( \nabla^2 J(u) \) is invertible.

**Proposition 4.7.** Let \( J: \Omega \to \mathbb{R} \) be a function defined on some open subset \( \Omega \subseteq \mathbb{R}^n \). If \( J \) is differentiable in \( \Omega \) and if some point \( u \in \Omega \) is a nondegenerate critical point such that \( \nabla^2 J(u) \) is positive definite, then \( J \) has a strict local minimum at \( u \).

**Remark:** It is possible to generalize Proposition 21.7 to infinite-dimensional spaces by finding a suitable generalization of the notion of a nondegenerate critical point. Firstly, we assume that \( E \) is a Banach space (a complete normed vector space). Then, we define the dual \( E' \) of \( E \) as the set of continuous linear forms on \( E \), so that \( E' = \mathcal{L}(E; \mathbb{R}) \). Following Lang, we use the notation \( E' \) for the space of continuous linear forms to avoid confusion with the space \( E^* = \text{Hom}(E, \mathbb{R}) \) of all linear maps from \( E \) to \( \mathbb{R} \). A continuous bilinear map \( \varphi: E \times E \to \mathbb{R} \) in \( L^2(E, E; \mathbb{R}) \) yields a map \( \Phi \) from \( E \) to \( E' \) given by

\[
\Phi(u) = \varphi_u,
\]

where \( \varphi_u \in E' \) is the linear form defined by

\[
\varphi_u(v) = \varphi(u, v).
\]

It is easy to check that \( \varphi_u \) is continuous and that the map \( \Phi \) is continuous. Then, we say that \( \varphi \) is nondegenerate iff \( \Phi: E \to E' \) is an isomorphism of Banach spaces, which means that \( \Phi \) is invertible and that both \( \Phi \) and \( \Phi^{-1} \) are continuous linear maps. Given a function \( J: \Omega \to \mathbb{R} \) differentiable on \( \Omega \) as before (where \( \Omega \) is an open subset of \( E \)), if \( D^2 J(u) \) exists for some \( u \in \Omega \), we say that \( u \) is a nondegenerate critical point if \( dJ(u) = 0 \) and if \( D^2 J(u) \) is nondegenerate. Of course, \( D^2 J(u) \) is positive definite if \( D^2 J(u)(w, w) > 0 \) for all \( w \in E - \{0\} \).

Using the above definition, Proposition 21.6 can be generalized to a nondegenerate positive definite bilinear form (on a Banach space) and Theorem 21.7 can also be generalized to the situation where \( J: \Omega \to \mathbb{R} \) is defined on an open subset of a Banach space. For details and proofs, see Cartan [26] (Part I Chapter 8) and Avez [7] (Chapter 8 and Chapter 10).

In the next section we make use of convexity; both on the domain \( \Omega \) and on the function \( J \) itself.

### 4.3 Using Convexity to Find Extrema

We begin by reviewing the definition of a convex set and of a convex function.
**Definition 4.4.** Given any real vector space \( E \), we say that a subset \( C \) of \( E \) is **convex** if either \( C = \emptyset \) or if for every pair of points \( u, v \in C \), the line segment connecting \( u \) and \( v \) is contained in \( C \), i.e.,

\[
(1 - \lambda)u + \lambda v \in C \quad \text{for all } \lambda \in \mathbb{R} \text{ such that } 0 \leq \lambda \leq 1.
\]

Given any two points \( u, v \in E \), the **line segment** \([u, v]\) is the set

\[
[u, v] = \{(1 - \lambda)u + \lambda v \in E \mid \lambda \in \mathbb{R}, 0 \leq \lambda \leq 1\}.
\]

Clearly, a nonempty set \( C \) is convex iff \([u, v] \subseteq C \) whenever \( u, v \in C \). See Figure 21.1 for an example of a convex set.

Figure 4.1: Figure (a) shows that a sphere is not convex in \( \mathbb{R}^3 \) since the dashed green line does not lie on its surface. Figure (b) shows that a solid ball is convex in \( \mathbb{R}^3 \).

**Definition 4.5.** If \( C \) is a nonempty convex subset of \( E \), a function \( f : C \rightarrow \mathbb{R} \) is **convex** (on \( C \)) if for every pair of points \( u, v \in C \),

\[
f((1 - \lambda)u + \lambda v) \leq (1 - \lambda)f(u) + \lambda f(v) \quad \text{for all } \lambda \in \mathbb{R} \text{ such that } 0 \leq \lambda \leq 1;
\]

the function \( f \) is **strictly convex** (on \( C \)) if for every pair of distinct points \( u, v \in C \) \( (u \neq v) \),

\[
f((1 - \lambda)u + \lambda v) < (1 - \lambda)f(u) + \lambda f(v) \quad \text{for all } \lambda \in \mathbb{R} \text{ such that } 0 < \lambda < 1;
\]

see Figure 21.2. The **epigraph**\(^1\) \( \text{epi}(f) \) of a function \( f : A \rightarrow \mathbb{R} \) defined on some subset \( A \) of \( \mathbb{R}^n \) is the subset of \( \mathbb{R}^{n+1} \) defined as

\[
\text{epi}(f) = \{(x, y) \in \mathbb{R}^{n+1} \mid f(x) \leq y, \ x \in A\}.
\]

\(^1\)“Epi” means above.
A function \( f : C \rightarrow \mathbb{R} \) defined on a convex subset \( C \) is \textit{concave} (resp. \textit{strictly concave}) if \((-f)\) is convex (resp. strictly convex).

It is obvious that a function \( f \) if convex iff its epigraph \( \text{epi}(f) \) is a convex subset of \( \mathbb{R}^{n+1} \).

![Graph of convex function](image_a)

![Graph of non-convex function](image_b)

Figure 4.2: Figures (a) and (b) are the graphs of real valued functions. Figure (a) is the graph of convex function since the blue line lies above the graph of \( f \). Figure (b) shows the graph of a function which is not convex.

Subspaces \( V \subseteq E \) of a vector space \( E \) are convex; \textit{affine subspaces}, that is, sets of the form \( u + V \), where \( V \) is a subspace of \( E \) and \( u \in E \), are convex. Balls (open or closed) are convex. Given any linear form \( \varphi \colon E \rightarrow \mathbb{R} \), for any scalar \( c \in \mathbb{R} \), the \textit{closed half–spaces}

\[
H_{\varphi,c}^+ = \{ u \in E \, | \, \varphi(u) \geq c \}, \quad H_{\varphi,c}^- = \{ u \in E \, | \, \varphi(u) \leq c \},
\]

are convex. Any intersection of half–spaces is convex. More generally, any intersection of convex sets is convex.

Linear forms are convex functions (but not strictly convex). Any norm \( \| \cdot \| : E \rightarrow \mathbb{R}_+ \) is a convex function. The max function,

\[
\max(x_1, \ldots, x_n) = \max\{x_1, \ldots, x_n\}
\]

is convex on \( \mathbb{R}^n \). The exponential \( x \mapsto e^{cx} \) is strictly convex for any \( c \neq 0 \ (c \in \mathbb{R}) \). The logarithm function is concave on \( \mathbb{R}_+ - \{0\} \), and the \textit{log-determinant function} \( \log \det \) is concave on the set of symmetric positive definite matrices. This function plays an important
role in convex optimization. An excellent exposition of convexity and its applications to optimization can be found in Boyd [22].

Here is a necessary condition for a function to have a local minimum with respect to a convex subset $U$.

**Theorem 4.8.** (Necessary condition for a local minimum on a convex subset) Let $J : \Omega \to \mathbb{R}$ be a function defined on some open subset $\Omega$ of a normed vector space $E$ and let $U \subseteq \Omega$ be a nonempty convex subset. Given any $u \in U$, if $dJ(u)$ exists and if $J$ has a local minimum in $u$ with respect to $U$, then

$$dJ(u)(v - u) \geq 0 \quad \text{for all } v \in U.$$ 

**Proof.** Let $v = u + w$ be an arbitrary point in $U$. Since $U$ is convex, we have $u + tw \in U$ for all $t$ such that $0 \leq t \leq 1$. Since $dJ(u)$ exists, we can write

$$J(u + tw) - J(u) = dJ(u)(tw) + \|tw\| \epsilon(tw)$$

with $\lim_{t \to 0} \epsilon(tw) = 0$. However, because $0 \leq t \leq 1$,

$$J(u + tw) - J(u) = t(dJ(u)(w) + \|w\| \epsilon(tw))$$

and since $u$ is a local minimum with respect to $U$, we have $J(u + tw) - J(u) \geq 0$, so we get

$$t(dJ(u)(w) + \|w\| \epsilon(tw)) \geq 0.$$ 

The above implies that $dJ(u)(w) \geq 0$, because otherwise we could pick $t > 0$ small enough so that

$$dJ(u)(w) + \|w\| \epsilon(tw) < 0,$$

a contradiction. Since the argument holds for all $v = u + w \in U$, the theorem is proved. \qed

Observe that the convexity of $U$ is a substitute for the use of Lagrange multipliers, but we now have to deal with an inequality instead of an equality.

Consider the special case where $U$ is a subspace of $E$. In this case since $u \in U$ we have $2u \in U$, and for any $u + w \in U$, we must have $2u - (u + w) = u - w \in U$. The previous theorem implies that $dJ(u)(w) \geq 0$ and $dJ(u)(-w) \geq 0$, that is, $dJ(u)(w) \leq 0$, so $dJ(u) = 0$. Since the argument holds for $w \in U$ (because $U$ is a subspace, if $u, w \in U$, then $u + w \in U$), we conclude that

$$dJ(u)(w) = 0 \quad \text{for all } w \in U.$$ 

We will now characterize convex functions when they have a first derivative or a second derivative.

**Proposition 4.9.** (Convexity and first derivative) Let $f : \Omega \to \mathbb{R}$ be a function differentiable on some open subset $\Omega$ of a normed vector space $E$ and let $U \subseteq \Omega$ be a nonempty convex subset.
(1) The function $f$ is convex on $U$ iff
\[ f(v) \geq f(u) + df(u)(v - u) \quad \text{for all } u, v \in U. \]

(2) The function $f$ is strictly convex on $U$ iff
\[ f(v) > f(u) + df(u)(v - u) \quad \text{for all } u, v \in U \text{ with } u \neq v. \]

See Figure 21.3.

Figure 4.3: An illustration of a convex valued function $f$. Since $f$ is convex it always lies above its tangent line.

Proof. Let $u, v \in U$ be any two distinct points and pick $\lambda \in \mathbb{R}$ with $0 < \lambda < 1$. If the function $f$ is convex, then
\[ f(((1 - \lambda)u + \lambda v) \leq (1 - \lambda)f(u) + \lambda f(v), \]
which yields
\[ \frac{f(((1 - \lambda)u + \lambda v) - f(u)}{\lambda} \leq f(v) - f(u). \]

It follows that
\[ df(u)(v - u) = \lim_{\lambda \to 0} \frac{f(((1 - \lambda)u + \lambda v) - f(u)}{\lambda} \leq f(v) - f(u). \]
If $f$ is strictly convex, the above reasoning does not work, because a strict inequality is not necessarily preserved by “passing to the limit.” We have recourse to the following trick: For any $\omega$ such that $0 < \omega < 1$, observe that

$$(1 - \lambda)u + \lambda v = u + \lambda(v - u) = \frac{\omega - \lambda}{\omega}u + \frac{\lambda}{\omega}(u + \omega(v - u)).$$

If we assume that $0 < \lambda \leq \omega$, the convexity of $f$ yields

$$f(u + \lambda(v - u)) \leq \frac{\omega - \lambda}{\omega}f(u) + \frac{\lambda}{\omega}f(u + \omega(v - u)).$$

If we subtract $f(u)$ to both sides, we get

$$\frac{f(u + \lambda(v - u)) - f(u)}{\lambda} \leq \frac{f(u + \omega(v - u)) - f(u)}{\omega}.$$

Now, since $0 < \omega < 1$ and $f$ is strictly convex,

$$f(u + \omega(v - u)) = f((1 - \omega)u + \omega v) < (1 - \omega)f(u) + \omega f(v),$$

which implies that

$$\frac{f(u + \omega(v - u)) - f(u)}{\omega} < f(v) - f(u),$$

and thus we get

$$\frac{f(u + \lambda(v - u)) - f(u)}{\lambda} \leq \frac{f(u + \omega(v - u)) - f(u)}{\omega} < f(v) - f(u).$$

If we let $\lambda$ go to 0, by passing to the limit we get

$$df(u)(v - u) \leq \frac{f(u + \omega(v - u)) - f(u)}{\omega} < f(v) - f(u),$$

which yields the desired strict inequality.

Let us now consider the converse of (1); that is, assume that

$$f(v) \geq f(u) + df(u)(v - u) \quad \text{for all } u, v \in U.$$

For any two distinct points $u, v \in U$ and for any $\lambda$ with $0 < \lambda < 1$, we get

$$f(v) \geq f(v + \lambda(v - u)) - \lambda df(v + \lambda(u - v))(u - v)$$

$$f(u) \geq f(v + \lambda(u - v)) + (1 - \lambda)df(v + \lambda(u - v))(u - v),$$

and if we multiply the first inequality by $1 - \lambda$ and the second inequality by $\lambda$ and then add up the resulting inequalities, we get

$$(1 - \lambda)f(v) + \lambda f(u) \geq f(v + \lambda(u - v)) = f((1 - \lambda)v + \lambda u),$$

which proves that $f$ is convex.

The proof of the converse of (2) is similar, except that the inequalities are replaced by strict inequalities.
We now establish a convexity criterion using the second derivative of $f$. This criterion is often easier to check than the previous one.

**Proposition 4.10.** (Convexity and second derivative) Let $f : \Omega \to \mathbb{R}$ be a function twice differentiable on some open subset $\Omega$ of a normed vector space $E$ and let $U \subseteq \Omega$ be a nonempty convex subset.

1. The function $f$ is convex on $U$ iff
   
   $$D^2f(u)(v-u, v-u) \geq 0 \quad \text{for all } u, v \in U.$$  

2. If
   
   $$D^2f(u)(v-u, v-u) > 0 \quad \text{for all } u, v \in U \text{ with } u \neq v,$$

   then $f$ is strictly convex.

**Proof.** First, assume that the inequality in Condition (1) is satisfied. For any two distinct points $u, v \in U$, the formula of Taylor–Maclaurin yields

$$f(v) - f(u) - df(u)(v-u) = \frac{1}{2}D^2f(w)(v-u, v-u) = \frac{\rho^2}{2}D^2f(w)(v-w, v-w),$$

for some $w = (1-\lambda)u + \lambda v = u + \lambda(v-u)$ with $0 < \lambda < 1$, and with $\rho = 1/(1-\lambda) > 0$, so that $v-u = \rho(v-w)$. Since $D^2f(u)(v-w, v-w) \geq 0$ for all $u, w \in U$, we conclude by applying Proposition 21.9(1).

Similarly, if (2) holds, the above reasoning and Proposition 21.9(2) imply that $f$ is strictly convex.

To prove the necessary condition in (1), define $g : \Omega \to \mathbb{R}$ by

$$g(v) = f(v) - df(u)(v),$$

where $u \in U$ is any point considered fixed. If $f$ is convex, since

$$g(v) - g(u) = f(v) - f(u) - df(u)(v-u),$$

Proposition 21.9 implies that $f(v) - f(u) - df(u)(v-u) \geq 0$, which implies that $g$ has a local minimum at $u$ with respect to all $v \in U$. Therefore, we have $dg(u) = 0$. Observe that $g$ is twice differentiable in $\Omega$ and $D^2g(u) = D^2f(u)$, so the formula of Taylor–Young yields for every $v = u + w \in U$ and all $t$ with $0 \leq t \leq 1$,

$$0 \leq g(u + tw) - g(u) = \frac{t^2}{2}D^2f(u)(tw, tw) + \|tw\|^2 \epsilon(tw) = \frac{t^2}{2}(D^2f(u)(w, w) + 2\|w\|^2 \epsilon(wt)),$$

with $\lim_{t \to 0} \epsilon(wt) = 0$, and for $t$ small enough, we must have $D^2f(u)(w, w) \geq 0$, as claimed.  \qed
The converse of Proposition 21.10 (2) is false as we see by considering the function $f$ given by $f(x) = x^4$.

**Example 4.1.** On the other hand, if $f$ is a quadratic function of the form

$$f(u) = \frac{1}{2} u^\top A u - u^\top b$$

where $A$ is a symmetric matrix, we know that

$$df(u)(v) = v^\top (Au - b),$$

so

$$f(v) - f(u) - df(u)(v - u) = \frac{1}{2} v^\top Av - v^\top b - \frac{1}{2} u^\top Au + u^\top b - (v - u)^\top (Au - b)$$

$$= \frac{1}{2} v^\top Av - \frac{1}{2} u^\top Au - (v - u)^\top Au$$

$$= \frac{1}{2} v^\top Av + \frac{1}{2} u^\top Au - v^\top Au$$

$$= \frac{1}{2} (v - u)^\top A(v - u).$$

Therefore, Proposition 21.9 implies that if $A$ is positive semidefinite, then $f$ is convex and if $A$ is positive definite, then $f$ is strictly convex. The converse follows by Proposition 21.10.

We conclude this section by applying our previous theorems to convex functions defined on convex subsets. In this case, local minima (resp. local maxima) are global minima (resp. global maxima).

**Definition 4.6.** Let $f : E \to \mathbb{R}$ be any function defined on some normed vector space (or more generally, any set). For any $u \in E$, we say that $f$ has a *minimum* in $u$ (resp. *maximum* in $u$) if

$$f(u) \leq f(v) \quad \text{(resp. } f(u) \geq f(v) \text{)} \quad \text{for all } v \in E.$$  

We say that $f$ has a *strict minimum* in $u$ (resp. *strict maximum* in $u$) if

$$f(u) < f(v) \quad \text{(resp. } f(u) > f(v) \text{)} \quad \text{for all } v \in E - \{u\}.$$  

If $U \subseteq E$ is a subset of $E$ and $u \in U$, we say that $f$ has a *minimum* in $u$ (resp. *strict minimum* in $u$) with respect to $U$ if

$$f(u) \leq f(v) \quad \text{for all } v \in U \quad \text{(resp. } f(u) < f(v) \quad \text{for all } v \in U - \{u\}),$$

and similarly for a *maximum* in $u$ (resp. *strict maximum* in $u$) with respect to $U$ with $\leq$ changed to $\geq$ and $<$ to $>$. 
Sometimes, we say *global* maximum (or minimum) to stress that a maximum (or a minimum) is not simply a local maximum (or minimum).

**Theorem 4.11.** Given any normed vector space $E$, let $U$ be any nonempty convex subset of $E$.

1. For any convex function $J: U \rightarrow \mathbb{R}$, for any $u \in U$, if $J$ has a local minimum at $u$ in $U$, then $J$ has a (global) minimum at $u$ in $U$.

2. Any strict convex function $J: U \rightarrow \mathbb{R}$ has at most one minimum (in $U$), and if it does, then it is a strict minimum (in $U$).

3. Let $J: \Omega \rightarrow \mathbb{R}$ be any function defined on some open subset $\Omega$ of $E$ with $U \subseteq \Omega$ and assume that $J$ is convex on $U$. For any point $u \in U$, if $dJ(u)$ exists, then $J$ has a minimum in $u$ with respect to $U$ iff

$$dJ(u)(v - u) \geq 0 \quad \text{for all } v \in U.$$ 

4. If the convex subset $U$ in (3) is open, then the above condition is equivalent to

$$dJ(u) = 0.$$

**Proof.** (1) Let $v = u + w$ be any arbitrary point in $U$. Since $J$ is convex, for all $t$ with $0 \leq t \leq 1$, we have

$$J(u + tw) = J(u + t(v - u)) \leq (1 - t)J(u) + tJ(v),$$

which yields

$$J(u + tw) - J(u) \leq t(J(v) - J(u)).$$

Because $J$ has a local minimum in $u$, there is some $t_0$ with $0 < t_0 < 1$ such that

$$0 \leq J(u + t_0w) - J(u),$$

which implies that $J(v) - J(u) \geq 0$.

(2) If $J$ is strictly convex, the above reasoning with $w \neq 0$ shows that there is some $t_0$ with $0 < t_0 < 1$ such that

$$0 \leq J(u + t_0w) - J(u) < t_0(J(v) - J(u)), $$

which shows that $u$ is a strict global minimum (in $U$), and thus that it is unique.

(3) We already know from Theorem 21.8 that the condition $dJ(u)(v - u) \geq 0$ for all $v \in U$ is necessary (even if $J$ is not convex). Conversely, because $J$ is convex, careful inspection of the proof of part (1) of Proposition 21.9 shows that only the fact that $dJ(u)$ exists in needed to prove that

$$J(v) - J(u) \geq dJ(u)(v - u) \quad \text{for all } v \in U,$$
and if
\[ dJ(u)(v - u) \geq 0 \quad \text{for all } v \in U, \]
then
\[ J(v) - J(u) \geq 0 \quad \text{for all } v \in U, \]
as claimed.

(4) If \( U \) is open, then for every \( u \in U \) we can find an open ball \( B \) centered at \( u \) of radius \( \epsilon \) small enough so that \( B \subseteq U \). Then, for any \( w \neq 0 \) such that \( \|w\| < \epsilon \), we have both \( v = u + w \in B \) and \( v' = u - w \in B \), so condition (3) implies that
\[ dJ(u)(w) \geq 0 \quad \text{and} \quad dJ(u)(-w) \geq 0, \]
which yields
\[ dJ(u)(w) = 0. \]
Since the above holds for all \( w \neq 0 \) such such that \( \|w\| < \epsilon \) and since \( dJ(u) \) is linear, we leave it to the reader to fill in the details of the proof that \( dJ(u) = 0 \).

Theorem 21.11 can be used to rederive the fact that the least squares solutions of a linear system \( Ax = b \) (where \( A \) is an \( m \times n \) matrix) are given by the normal equation
\[ A^\top Ax = A^\top b. \]
For this, we consider the quadratic function
\[ J(v) = \frac{1}{2} \|Av - b\|_2^2 - \frac{1}{2} \|b\|_2^2, \]
and our least squares problem is equivalent to finding the minima of \( J \) on \( \mathbb{R}^n \). A computation reveals that
\[ J(v) = \frac{1}{2} \|Av - b\|_2^2 - \frac{1}{2} \|b\|_2^2 \]
\[ = \frac{1}{2} (Av - b)^\top (Av - b) - \frac{1}{2} b^\top b \]
\[ = \frac{1}{2} (v^\top A^\top - b^\top)(Av - b) - \frac{1}{2} b^\top b \]
\[ = \frac{1}{2} v^\top A^\top Av - v^\top A^\top b, \]
and so
\[ dJ(u) = A^\top Au - A^\top b. \]
Since \( A^\top A \) is positive semidefinite, the function \( J \) is convex, and Theorem 21.11(4) implies that the minima of \( J \) are the solutions of the equation
\[ A^\top Au - A^\top b = 0. \]
The considerations in this chapter reveal the need to find methods for finding the zeros of the derivative map
\[ dJ : \Omega \rightarrow E', \]
where \( \Omega \) is some open subset of a normed vector space \( E \) and \( E' \) is the space of all continuous linear forms on \( E \) (a subspace of \( E^* \)). Generalizations of Newton’s method yield such methods and they are the objet of the next chapter.

4.4 Summary

The main concepts and results of this chapter are listed below:

- Local minimum, local maximum, local extremum, strict local minimum, strict local maximum.
- Necessary condition for a local extremum involving the derivative; critical point.
- Local minimum with respect to a subset \( U \), local maximum with respect to a subset \( U \), local extremum with respect to a subset \( U \).
- Constrained local extremum.
- Necessary condition for a constrained extremum.
- Necessary condition for a constrained extremum in terms of Lagrange multipliers.
- Lagrangian.
- Critical points of a Lagrangian.
- Necessary condition of an unconstrained local minimum involving the second-order derivative.
- Sufficient condition for a local minimum involving the second-order derivative.
- A sufficient condition involving nondegenerate critical points.
- Convex sets, convex functions, concave functions, strictly convex functions, strictly concave functions.
- Necessary condition for a local minimum on a convex set involving the derivative.
- Convexity of a function involving a condition on its first derivative.
- Convexity of a function involving a condition on its second derivative.
- Minima of convex functions on convex sets.
Chapter 5

Newton’s Method and Its Generalizations

5.1 Newton’s Method for Real Functions of a Real Argument

In Chapter 21 we investigated the problem of determining when a function $J: \Omega \to \mathbb{R}$ defined on some open subset $\Omega$ of a normed vector space $E$ has a local extremum. Proposition 21.1 gives a necessary condition when $J$ is differentiable: if $J$ has a local extremum at $u \in \Omega$, then we must have

$$J'(u) = 0.$$ 

Thus we are led to the problem of finding the zeros of the derivative

$$J': \Omega \to E',$$

where $E' = \mathcal{L}(E; \mathbb{R})$ is the set of linear continuous functions from $E$ to $\mathbb{R}$; that is, the dual of $E$, as defined in the remark after Proposition 21.7.

This leads us to consider the problem in a more general form, namely: Given a function $f: \Omega \to Y$ from an open subset $\Omega$ of a normed vector space $X$ to a normed vector space $Y$, find

(i) Sufficient conditions which guarantee the existence of a zero of the function $f$; that is, an element $a \in \Omega$ such that $f(a) = 0$.

(ii) An algorithm for approximating such an $a$, that is, a sequence $(x_k)$ of points of $\Omega$ whose limit is $a$.

When $X = Y = \mathbb{R}$, we can use Newton’s method. We pick some initial element $x_0 \in \mathbb{R}$ “close enough” to a zero $a$ of $f$, and we define the sequence $(x_k)$ by

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)},$$

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for all \( k \geq 0 \), provided that \( f'(x_k) \neq 0 \). The idea is to define \( x_{k+1} \) as the intersection of the \( x \)-axis with the tangent line to the graph of the function \( x \mapsto f(x) \) at the point \((x_k, f(x_k))\). Indeed, the equation of this tangent line is
\[
y - f(x_k) = f'(x_k)(x - x_k),
\]
and its intersection with the \( x \)-axis is obtained for \( y = 0 \), which yields
\[
x = x_k - \frac{f(x_k)}{f'(x_k)};
\]
as claimed.

For example, if \( \alpha > 0 \) and \( f(x) = x^2 - \alpha \), Newton’s method yields the sequence
\[
x_{k+1} = \frac{1}{2} \left( x_k + \frac{\alpha}{x_k} \right)
\]
to compute the square root \( \sqrt{\alpha} \) of \( \alpha \). It can be shown that the method converges to \( \sqrt{\alpha} \) for any \( x_0 > 0 \). Actually, the method also converges when \( x_0 < 0 \)! Find out what is the limit.

The case of a real function suggests the following method for finding the zeros of a function \( f: \Omega \to Y \), with \( \Omega \subseteq X \): given a starting point \( x_0 \in \Omega \), the sequence \((x_k)\) is defined by
\[
x_{k+1} = x_k - (f'(x_k))^{-1}(f(x_k))
\]
for all \( k \geq 0 \).

For the above to make sense, it must be ensured that

1. All the points \( x_k \) remain within \( \Omega \).
2. The function \( f \) is differentiable within \( \Omega \).
3. The derivative \( f'(x) \) is a bijection from \( X \) to \( Y \) for all \( x \in \Omega \).

These are rather demanding conditions but there are sufficient conditions that guarantee that they are met. Another practical issue is that it may be very costly to compute \((f'(x_k))^{-1}\) at every iteration step. In the next section, we investigate generalizations of Newton’s method which address the issues that we just discussed.

### 5.2 Generalizations of Newton’s Method

Suppose that \( f: \Omega \to \mathbb{R}^n \) is given by \( n \) functions \( f_i: \Omega \to \mathbb{R} \), where \( \Omega \subseteq \mathbb{R}^n \). In this case, finding a zero \( a \) of \( f \) is equivalent to solving the system
\[
\begin{align*}
f_1(a_1, \ldots, a_n) &= 0 \\
f_2(a_1, \ldots, a_n) &= 0 \\
& \vdots \\
f_n(a_1, \ldots, a_n) &= 0.
\end{align*}
\]
A single iteration of Newton’s method consists in solving the linear system

\[(J(f)(x_k))\epsilon_k = -f(x_k),\]

and then setting

\[x_{k+1} = x_k + \epsilon_k,\]

where \(J(f)(x_k) = \left(\frac{\partial f_i}{\partial x_j}(x_k)\right)\) is the Jacobian matrix of \(f\) at \(x_k\).

In general, it is very costly to compute \(J(f)(x_k)\) at each iteration and then to solve the corresponding linear system. If the method converges, the consecutive vectors \(x_k\) should differ only a little, as also the corresponding matrices \(J(f)(x_k)\). Thus, we are led to a variant of Newton’s method which consists in keeping the same matrix for \(p\) consecutive steps (where \(p\) is some fixed integer \(\geq 2\)):

\[
\begin{align*}
x_{k+1} &= x_k - (f'(x_0))^{-1}(f(x_k)), & 0 \leq k \leq p - 1 \\
x_{k+1} &= x_k - (f'(x_p))^{-1}(f(x_k)), & p \leq k \leq 2p - 1 \\
\vdots
\end{align*}
\]

\[
\begin{align*}
x_{k+1} &= x_k - (f'(x_{rp}))^{-1}(f(x_k)), & rp \leq k \leq (r + 1)p - 1 \\
\vdots
\end{align*}
\]

It is also possible to set \(p = \infty\), that is, to use the same matrix \(f'(x_0)\) for all iterations, which leads to iterations of the form

\[x_{k+1} = x_k - (f'(x_0))^{-1}(f(x_k)), \quad k \geq 0,\]

or even to replace \(f'(x_0)\) by a particular matrix \(A_0\) which is easy to invert:

\[x_{k+1} = x_k - A_0^{-1}f(x_k), \quad k \geq 0.\]

In the last two cases, if possible, we use an LU factorization of \(f'(x_0)\) or \(A_0\) to speed up the method. In some cases, it may even possible to set \(A_0 = I\).

The above considerations lead us to the definition of a generalized Newton method, as in Ciarlet [30] (Chapter 7). Recall that a linear map \(f \in \mathcal{L}(E; F)\) is called an isomorphism iff \(f\) is continuous, bijective, and \(f^{-1}\) is also continuous.

**Definition 5.1.** If \(X\) and \(Y\) are two normed vector spaces and if \(f: \Omega \to Y\) is a function from some open subset \(\Omega\) of \(X\), a generalized Newton method for finding zeros of \(f\) consists of

1. A sequence of families \((A_k(x))\) of linear isomorphisms from \(X\) to \(Y\), for all \(x \in \Omega\) and all integers \(k \geq 0\);

2. Some starting point \(x_0 \in \Omega\);
(3) A sequence \((x_k)\) of points of \(\Omega\) defined by
\[
x_{k+1} = x_k - (A_k(x_\ell))^{-1}(f(x_k)), \quad k \geq 0,
\]
where for every integer \(k \geq 0\), the integer \(\ell\) satisfies the condition
\[
0 \leq \ell \leq k.
\]

The function \(A_k(x)\) usually depends on \(f'\).

Definition 22.1 gives us enough flexibility to capture all the situations that we have previously discussed:
\[
\begin{align*}
A_k(x) &= f'(x), \quad \ell = k \\
A_k(x) &= f'(x), \quad \ell = \min\{rp, k\}, \text{ if } rp \leq k \leq (r + 1)p - 1, r \geq 0 \\
A_k(x) &= f'(x), \quad \ell = 0 \\
A_k(x) &= A_0,
\end{align*}
\]
where \(A_0\) is a linear isomorphism from \(X\) to \(Y\). The first case corresponds to Newton’s original method and the others to the variants that we just discussed. We could also have \(A_k(x) = A_k\), a fixed linear isomorphism independent of \(x \in \Omega\).

The following theorem inspired by the Newton–Kantorovich theorem gives sufficient conditions that guarantee that the sequence \((x_k)\) constructed by a generalized Newton method converges to a zero of \(f\) close to \(x_0\). Although quite technical, these conditions are not very surprising.

**Theorem 5.1.** Let \(X\) be a Banach space, let \(f : \Omega \to Y\) be differentiable on the open subset \(\Omega \subseteq X\), and assume that there are constants \(r, M, \beta > 0\) such that if we let
\[
B = \{x \in X \mid \|x - x_0\| \leq r\} \subseteq \Omega,
\]
them
\[
(1) \quad \sup_{k \geq 0} \sup_{x \in B} \|A_k^{-1}(x)\|_{\mathcal{L}(Y,X)} \leq M,
\]
\[
(2) \quad \beta < 1 \text{ and } \sup_{k \geq 0} \sup_{x,x' \in B} \|f'(x) - A_k(x')\|_{\mathcal{L}(X,Y)} \leq \frac{\beta}{M}
\]
\[
(3) \quad \|f(x_0)\| \leq \frac{r}{M}(1 - \beta).
\]
Then, the sequence \((x_k)\) defined by
\[
x_{k+1} = x_k - A_k^{-1}(x_\ell)(f(x_k)), \quad 0 \leq \ell \leq k
\]
is entirely contained within \(B\) and converges to a zero \(a\) of \(f\), which is the only zero of \(f\) in \(B\). Furthermore, the convergence is geometric, which means that
\[
\|x_k - a\| \leq \frac{\|x_1 - x_0\| \beta^k}{1 - \beta},
\]
for some \(\beta < 1\).

A proof of Theorem 22.1 can be found in Ciarlet [30] (Section 7.5). It is not really difficult but quite technical.

If we assume that we already know that some element \(a \in \Omega\) is a zero of \(f\), the next theorem gives sufficient conditions for a special version of a generalized Newton method to converge. For this special method, the linear isomorphisms \(A_k(x)\) are independent of \(x \in \Omega\).

**Theorem 5.2.** Let \(X\) be a Banach space, and let \(f: \Omega \to Y\) be differentiable on the open subset \(\Omega \subseteq X\). If \(a \in \Omega\) is a point such that \(f(a) = 0\), if \(f'(a)\) is a linear isomorphism, and if there is some \(\lambda\) with \(0 < \lambda < 1/2\) such that

\[
\sup_{k \geq 0} \|A_k - f'(a)\|_{\mathcal{L}(X;Y)} \leq \frac{\lambda}{\|(f'(a))^{-1}\|_{\mathcal{L}(Y;X)}},
\]
then there is a closed ball \(B\) of center \(a\) such that for every \(x_0 \in B\), the sequence \((x_k)\) defined by
\[
x_{k+1} = x_k - A_k^{-1}(f(x_k)), \quad k \geq 0,
\]
is entirely contained within \(B\) and converges to \(a\), which is the only zero of \(f\) in \(B\). Furthermore, the convergence is geometric, which means that
\[
\|x_k - a\| \leq \beta^k \|x_0 - a\|,
\]
for some \(\beta < 1\).

A proof of Theorem 22.2 can be also found in Ciarlet [30] (Section 7.5).

For the sake of completeness, we state a version of the Newton–Kantorovich theorem, which corresponds to the case where \(A_k(x) = f'(x)\). In this instance, a stronger result can be obtained especially regarding upper bounds, and we state a version due to Gragg and Tapia which appears in Problem 7.5-4 of Ciarlet [30].

**Theorem 5.3.** (Newton–Kantorovich) Let \(X\) be a Banach space, and let \(f: \Omega \to Y\) be differentiable on the open subset \(\Omega \subseteq X\). Assume that there exist three positive constants \(\lambda, \mu, \nu\) and a point \(x_0 \in \Omega\) such that
\[
0 < \lambda \mu \nu \leq \frac{1}{2},
\]
and if we let
\[
\rho^- = \frac{1 - \sqrt{1 - 2\lambda\mu\nu}}{\mu\nu},
\]
\[
\rho^+ = \frac{1 + \sqrt{1 - 2\lambda\mu\nu}}{\mu\nu},
\]
\[
B = \{x \in X \mid \|x - x_0\| < \rho^-\}
\]
\[
\Omega^+ = \{x \in \Omega \mid \|x - x_0\| < \rho^+\},
\]
then \(\overline{B} \subseteq \Omega\), \(f'(x_0)\) is an isomorphism of \(\mathcal{L}(X;Y)\), and
\[
\|(f'(x_0))^{-1}\| \leq \mu,
\]
\[
\|(f'(x_0))^{-1}f(x_0)\| \leq \lambda,
\]
\[
\sup_{x,y \in \Omega^+} \|f'(x) - f'(y)\| \leq \nu \|x - y\|.
\]

Then, \(f'(x)\) is isomorphism of \(\mathcal{L}(X;Y)\) for all \(x \in B\), and the sequence defined by
\[
x_{k+1} = x_k - (f'(x_k))^{-1}(f(x_k)), \quad k \geq 0
\]
is entirely contained within the ball \(B\) and converges to a zero \(a\) of \(f\) which is the only zero of \(f\) in \(\Omega^+\). Finally, if we write \(\theta = \rho^- / \rho^+\), then we have the following bounds:
\[
\|x_k - a\| \leq \frac{2\sqrt{1 - 2\lambda\mu\nu}}{\lambda\mu\nu} \frac{\theta^{2k}}{1 - \theta^{2k}} \|x_1 - x_0\| \quad \text{if } \lambda\mu\nu < \frac{1}{2}
\]
\[
\|x_k - a\| \leq \frac{\|x_1 - x_0\|}{2^{k-1}} \quad \text{if } \lambda\mu\nu = \frac{1}{2},
\]
and
\[
\frac{2\|x_{k+1} - x_k\|}{1 + \sqrt{1 + 4\theta^{2k}(1 + \theta^{2k})^{-2}}} \leq \|x_k - a\| \leq \theta^{2k-1} \|x_k - x_{k-1}\|.
\]

We can now specialize Theorems 22.1 and 22.2 to the search of zeros of the derivative \(f'\): \(\Omega \to E'\), of a function \(f\): \(\Omega \to \mathbb{R}\), with \(\Omega \subseteq E\). The second derivative \(J''\) of \(J\) is a continuous bilinear form \(J'': E \times E \to \mathbb{R}\), but is is convenient to view it as a linear map in \(\mathcal{L}(E,E')\); the continuous linear form \(J''(u)\) is given by \(J''(u)(v) = J''(u,v)\). In our next theorem, we assume that the \(A_k(x)\) are isomorphisms in \(\mathcal{L}(E,E')\).

**Theorem 5.4.** Let \(E\) be a Banach space, let \(J: \Omega \to \mathbb{R}\) be twice differentiable on the open subset \(\Omega \subseteq E\), and assume that there are constants \(r, M, \beta > 0\) such that if we let
\[
B = \{x \in E \mid \|x - x_0\| \leq r\} \subseteq \Omega,
\]
then
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(1) \[ \sup_{k \geq 0} \sup_{x \in B} \| A_k^{-1}(x) \|_{\mathcal{L}(E';E)} \leq M, \]

(2) \[ \beta < 1 \text{ and } \sup_{k \geq 0} \sup_{x,x' \in B} \| J''(x) - A_k(x') \|_{\mathcal{L}(E;E')} \leq \frac{\beta}{M} \]

(3) \[ \| J'(x_0) \| \leq \frac{r}{M}(1 - \beta). \]

Then, the sequence \((x_k)\) defined by

\[ x_{k+1} = x_k - A_k^{-1}(x_\ell)(J'(x_k)), \quad 0 \leq \ell \leq k \]

is entirely contained within \(B\) and converges to a zero \(a\) of \(J'\), which is the only zero of \(J'\) in \(B\). Furthermore, the convergence is geometric, which means that

\[ \| x_k - a \| \leq \beta^k \| x_0 - a \|. \]

In the next theorem, we assume that the \(A_k(x)\) are isomorphisms in \(\mathcal{L}(E,E')\) that are independent of \(x \in \Omega\).

**Theorem 5.5.** Let \(E\) be a Banach space, and let \(J: \Omega \to \mathbb{R}\) be twice differentiable on the open subset \(\Omega \subseteq E\). If \(a \in \Omega\) is a point such that \(J'(a) = 0\), if \(J''(a)\) is a linear isomorphism, and if there is some \(\lambda\) with \(0 < \lambda < 1/2\) such that

\[ \sup_{k \geq 0} \| A_k - J''(a) \|_{\mathcal{L}(E;E')} \leq \frac{\lambda}{\| (J''(a))^{-1} \|_{\mathcal{L}(E';E)}}, \]

then there is a closed ball \(B\) of center \(a\) such that for every \(x_0 \in B\), the sequence \((x_k)\) defined by

\[ x_{k+1} = x_k - A_k^{-1}(J'(x_k)), \quad k \geq 0, \]

is entirely contained within \(B\) and converges to \(a\), which is the only zero of \(J'\) in \(B\). Furthermore, the convergence is geometric, which means that

\[ \| x_k - a \| \leq \beta^k \| x_0 - a \|, \]

for some \(\beta < 1\).

When \(E = \mathbb{R}^n\), the Newton method given by Theorem 22.4 yield an iteration step of the form

\[ x_{k+1} = x_k - A_k^{-1}(x_\ell) \nabla J(x_k), \quad 0 \leq \ell \leq k, \]
where $\nabla J(x_k)$ is the gradient of $J$ at $x_k$ (here, we identify $E'$ with $\mathbb{R}^n$). In particular, Newton’s original method picks $A_k = J''$, and the iteration step is of the form

$$x_{k+1} = x_k - (\nabla^2 J(x_k))^{-1}\nabla J(x_k), \quad k \geq 0,$$

where $\nabla^2 J(x_k)$ is the Hessian of $J$ at $x_k$.

As remarked in Ciarlet [30] (Section 7.5), generalized Newton methods have a very wide range of applicability. For example, various versions of gradient descent methods can be viewed as instances of Newton method.

Newton’s method also plays an important role in convex optimization, in particular, interior-point methods. A variant of Newton’s method dealing with equality constraints has been developed. We refer the reader to Boyd and Vandenberghe [22], Chapters 10 and 11, for a comprehensive exposition of these topics.

### 5.3 Summary

The main concepts and results of this chapter are listed below:

- Newton’s method for functions $f: \mathbb{R} \to \mathbb{R}$.
- Generalized Newton methods.
- The Newton-Kantorovich theorem.
Chapter 6

Quadratic Optimization Problems

6.1 Quadratic Optimization: The Positive Definite Case

In this chapter, we consider two classes of quadratic optimization problems that appear frequently in engineering and in computer science (especially in computer vision):

1. Minimizing

\[ Q(x) = \frac{1}{2} x^\top A x - x^\top b \]

over all \( x \in \mathbb{R}^n \), or subject to linear or affine constraints.

2. Minimizing

\[ Q(x) = \frac{1}{2} x^\top A x - x^\top b \]

over the unit sphere.

In both cases, \( A \) is a symmetric matrix. We also seek necessary and sufficient conditions for \( f \) to have a global minimum.

Many problems in physics and engineering can be stated as the minimization of some energy function, with or without constraints. Indeed, it is a fundamental principle of mechanics that nature acts so as to minimize energy. Furthermore, if a physical system is in a stable state of equilibrium, then the energy in that state should be minimal. For example, a small ball placed on top of a sphere is in an unstable equilibrium position. A small motion causes the ball to roll down. On the other hand, a ball placed inside and at the bottom of a sphere is in a stable equilibrium position, because the potential energy is minimal.

The simplest kind of energy function is a quadratic function. Such functions can be conveniently defined in the form

\[ Q(x) = x^\top A x - x^\top b, \]
where \( A \) is a symmetric \( n \times n \) matrix, and \( x, b \), are vectors in \( \mathbb{R}^n \), viewed as column vectors. Actually, for reasons that will be clear shortly, it is preferable to put a factor \( \frac{1}{2} \) in front of the quadratic term, so that

\[
Q(x) = \frac{1}{2} x^\top A x - x^\top b.
\]

The question is, under what conditions (on \( A \)) does \( Q(x) \) have a global minimum, preferably unique?

We give a complete answer to the above question in two stages:

1. In this section, we show that if \( A \) is symmetric positive definite, then \( Q(x) \) has a unique global minimum precisely when

\[
Ax = b.
\]

2. In Section 23.2, we give necessary and sufficient conditions in the general case, in terms of the pseudo-inverse of \( A \).

We begin with the matrix version of Definition 16.2 (Vol. I).

**Definition 6.1.** A symmetric positive definite matrix is a matrix whose eigenvalues are strictly positive, and a symmetric positive semidefinite matrix is a matrix whose eigenvalues are nonnegative.

Equivalent criteria are given in the following proposition.

**Proposition 6.1.** Given any Euclidean space \( E \) of dimension \( n \), the following properties hold:

1. Every self-adjoint linear map \( f : E \to E \) is positive definite iff

\[
\langle f(x), x \rangle > 0
\]

for all \( x \in E \) with \( x \neq 0 \).

2. Every self-adjoint linear map \( f : E \to E \) is positive semidefinite iff

\[
\langle f(x), x \rangle \geq 0
\]

for all \( x \in E \).

**Proof.** (1) First, assume that \( f \) is positive definite. Recall that every self-adjoint linear map has an orthonormal basis \( (e_1, \ldots, e_n) \) of eigenvectors, and let \( \lambda_1, \ldots, \lambda_n \) be the corresponding eigenvalues. With respect to this basis, for every \( x = x_1 e_1 + \cdots + x_n e_n \neq 0 \), we have

\[
\langle f(x), x \rangle = \langle f\left( \sum_{i=1}^{n} x_i e_i \right), \sum_{i=1}^{n} x_i e_i \rangle = \left( \sum_{i=1}^{n} \lambda_i x_i e_i, \sum_{i=1}^{n} x_i e_i \right) = \sum_{i=1}^{n} \lambda_i x_i^2,
\]
which is strictly positive, since \( \lambda_i > 0 \) for \( i = 1, \ldots, n \), and \( x_i^2 > 0 \) for some \( i \), since \( x \neq 0 \).

Conversely, assume that

\[ \langle f(x), x \rangle > 0 \]

for all \( x \neq 0 \). Then for \( x = e_i \), we get

\[ \langle f(e_i), e_i \rangle = \langle \lambda_i e_i, e_i \rangle = \lambda_i, \]

and thus \( \lambda_i > 0 \) for all \( i = 1, \ldots, n \).

(2) As in (1), we have

\[ \langle f(x), x \rangle = \sum_{i=1}^{n} \lambda_i x_i^2, \]

and since \( \lambda_i \geq 0 \) for \( i = 1, \ldots, n \) because \( f \) is positive semidefinite, we have \( \langle f(x), x \rangle \geq 0 \), as claimed. The converse is as in (1) except that we get only \( \lambda_i \geq 0 \) since \( \langle f(e_i), e_i \rangle \geq 0 \).

Some special notation is customary (especially in the field of convex optimization) to express that a symmetric matrix is positive definite or positive semidefinite.

**Definition 6.2.** Given any \( n \times n \) symmetric matrix \( A \) we write \( A \succeq 0 \) if \( A \) is positive semidefinite and we write \( A \succ 0 \) if \( A \) is positive definite.

It should be noted that we can define the relation

\[ A \succeq B \]

between any two \( n \times n \) matrices (symmetric or not) iff \( A - B \) is symmetric positive semidefinite. It is easy to check that this relation is actually a partial order on matrices, called the **positive semidefinite cone ordering**; for details, see Boyd and Vandenberghe [22], Section 2.4.

If \( A \) is symmetric positive definite, it is easily checked that \( A^{-1} \) is also symmetric positive definite. Also, if \( C \) is a symmetric positive definite \( m \times m \) matrix and \( A \) is an \( m \times n \) matrix of rank \( n \) (and so \( m \geq n \) and the map \( x \mapsto Ax \) is surjective onto \( \mathbb{R}^m \)), then \( A^\top CA \) is symmetric positive definite.

We can now prove that

\[ Q(x) = \frac{1}{2} x^\top Ax - x^\top b \]

has a global minimum when \( A \) is symmetric positive definite.

**Proposition 6.2.** Given a quadratic function

\[ Q(x) = \frac{1}{2} x^\top Ax - x^\top b, \]

if \( A \) is symmetric positive definite, then \( Q(x) \) has a unique global minimum for the solution of the linear system \( Ax = b \). The minimum value of \( Q(x) \) is

\[ Q(A^{-1}b) = -\frac{1}{2} b^\top A^{-1}b. \]
Proof. Since $A$ is positive definite, it is invertible, since its eigenvalues are all strictly positive. Let $x = A^{-1}b$, and compute $Q(y) - Q(x)$ for any $y \in \mathbb{R}^n$. Since $Ax = b$, we get

$$
Q(y) - Q(x) = \frac{1}{2} y^\top Ay - y^\top b - \frac{1}{2} x^\top Ax + x^\top b
= \frac{1}{2} y^\top Ay - y^\top Ax + \frac{1}{2} x^\top Ax
= \frac{1}{2} (y - x)^\top A(y - x).
$$

Since $A$ is positive definite, the last expression is nonnegative, and thus

$$
Q(y) \geq Q(x)
$$

for all $y \in \mathbb{R}^n$, which proves that $x = A^{-1}b$ is a global minimum of $Q(x)$. A simple computation yields

$$
Q(A^{-1}b) = -\frac{1}{2} b^\top A^{-1}b.
$$

Remarks:

(1) The quadratic function $Q(x)$ is also given by

$$
Q(x) = \frac{1}{2} x^\top Ax - b^\top x,
$$

but the definition using $x^\top b$ is more convenient for the proof of Proposition 23.2.

(2) If $Q(x)$ contains a constant term $c \in \mathbb{R}$, so that

$$
Q(x) = \frac{1}{2} x^\top Ax - x^\top b + c,
$$

the proof of Proposition 23.2 still shows that $Q(x)$ has a unique global minimum for $x = A^{-1}b$, but the minimal value is

$$
Q(A^{-1}b) = -\frac{1}{2} b^\top A^{-1}b + c.
$$

Thus, when the energy function $Q(x)$ of a system is given by a quadratic function

$$
Q(x) = \frac{1}{2} x^\top Ax - x^\top b,
$$

where $A$ is symmetric positive definite, finding the global minimum of $Q(x)$ is equivalent to solving the linear system $Ax = b$. Sometimes, it is useful to recast a linear problem $Ax = b$
6.1. QUADRATIC OPTIMIZATION: THE POSITIVE DEFINITE CASE

as a variational problem (finding the minimum of some energy function). However, very often, a minimization problem comes with extra constraints that must be satisfied for all admissible solutions. For instance, we may want to minimize the quadratic function

\[ Q(x_1, x_2) = \frac{1}{2} (x_1^2 + x_2^2) \]

subject to the constraint

\[ 2x_1 - x_2 = 5. \]

The solution for which \( Q(x_1, x_2) \) is minimum is no longer \((x_1, x_2) = (0, 0)\), but instead, \((x_1, x_2) = (2, -1)\), as will be shown later.

Geometrically, the graph of the function defined by \( z = Q(x_1, x_2) \) in \( \mathbb{R}^3 \) is a paraboloid of revolution \( P \) with axis of revolution \( OZ \). The constraint

\[ 2x_1 - x_2 = 5 \]

corresponds to the vertical plane \( H \) parallel to the \( z \)-axis and containing the line of equation \( 2x_1 - x_2 = 5 \) in the \( xy \)-plane. Thus, the constrained minimum of \( Q \) is located on the parabola that is the intersection of the paraboloid \( P \) with the plane \( H \).

A nice way to solve constrained minimization problems of the above kind is to use the method of Lagrange multipliers discussed in Section 21.1. But first, let us define precisely what kind of minimization problems we intend to solve.

**Definition 6.3.** The quadratic constrained minimization problem consists in minimizing a quadratic function

\[ Q(x) = \frac{1}{2} x^\top A^{-1} x - b^\top x \]

subject to the linear constraints

\[ B^\top x = f, \]

where \( A^{-1} \) is an \( m \times m \) symmetric positive definite matrix, \( B \) is an \( m \times n \) matrix of rank \( n \) (so that \( m \geq n \)), and where \( b, x \in \mathbb{R}^m \) (viewed as column vectors), and \( f \in \mathbb{R}^n \) (viewed as a column vector).

The reason for using \( A^{-1} \) instead of \( A \) is that the constrained minimization problem has an interpretation as a set of equilibrium equations in which the matrix that arises naturally is \( A \) (see Strang [102]). Since \( A \) and \( A^{-1} \) are both symmetric positive definite, this doesn’t make any difference, but it seems preferable to stick to Strang’s notation.

As explained in Section 21.1, the method of Lagrange multipliers consists in incorporating the \( n \) constraints \( B^\top x = f \) into the quadratic function \( Q(x) \), by introducing extra variables \( \lambda = (\lambda_1, \ldots, \lambda_n) \) called Lagrange multipliers, one for each constraint. We form the Lagrangian

\[ L(x, \lambda) = Q(x) + \lambda^\top (B^\top x - f) = \frac{1}{2} x^\top A^{-1} x - (b - B\lambda)^\top x - \lambda^\top f. \]
We know from Theorem 21.3 that a necessary condition for our constrained optimization problem to have a solution is that \( \nabla L(x, \lambda) = 0 \). Since
\[
\begin{align*}
\frac{\partial L}{\partial x}(x, \lambda) &= A^{-1}x - (b - B\lambda) \\
\frac{\partial L}{\partial \lambda}(x, \lambda) &= B^T x - f,
\end{align*}
\]
we obtain the system of linear equations
\[
\begin{align*}
A^{-1}x + B\lambda &= b, \\
B^T x &= f,
\end{align*}
\]
which can be written in matrix form as
\[
\begin{pmatrix} A^{-1} & B \\ B^T & 0 \end{pmatrix} \begin{pmatrix} x \\ \lambda \end{pmatrix} = \begin{pmatrix} b \\ f \end{pmatrix}.
\]
We shall prove in Proposition 23.3 below that our constrained minimization problem has a unique solution actually given by the above system.

Note that the matrix of this system is symmetric. We solve it as follows. Eliminating \( x \) from the first equation
\[
A^{-1}x + B\lambda = b,
\]
we get
\[
x = A(b - B\lambda),
\]
and substituting into the second equation, we get
\[
B^T A(b - B\lambda) = f,
\]
that is,
\[
B^T AB\lambda = B^T Ab - f.
\]
However, by a previous remark, since \( A \) is symmetric positive definite and the columns of \( B \) are linearly independent, \( B^T AB \) is symmetric positive definite, and thus invertible. Thus we obtain the solution
\[
\lambda = (B^T AB)^{-1}(B^T Ab - f), \quad x = A(b - B\lambda).
\]
Note that this way of solving the system requires solving for the Lagrange multipliers first.

Letting \( e = b - B\lambda \), we also note that the system
\[
\begin{pmatrix} A^{-1} & B \\ B^T & 0 \end{pmatrix} \begin{pmatrix} x \\ \lambda \end{pmatrix} = \begin{pmatrix} b \\ f \end{pmatrix}
\]
is equivalent to the system
\[ \begin{align*}
  e &= b - B\lambda, \\
  x &= Ae, \\
  B^\top x &= f.
\end{align*} \]

The latter system is called the \textit{equilibrium equations} by Strang [102]. Indeed, Strang shows that the equilibrium equations of many physical systems can be put in the above form. This includes spring-mass systems, electrical networks, and trusses, which are structures built from elastic bars. In each case, \( x, e, b, A, \lambda, f \), and \( K = B^\top AB \) have a physical interpretation. The matrix \( K = B^\top AB \) is usually called the \textit{stiffness matrix}. Again, the reader is referred to Strang [102].

In order to prove that our constrained minimization problem has a unique solution, we proceed to prove that the constrained minimization of \( Q(x) \) subject to \( B^\top x = f \) is equivalent to the unconstrained maximization of another function \( -G(\lambda) \). We get \( G(\lambda) \) by minimizing the Lagrangian \( L(x, \lambda) \) treated as a function of \( x \) alone. The function \( -G(\lambda) \) is the \textit{dual function} of the Lagrangian \( L(x, \lambda) \). Here we are encountering a special case of the notion of dual function defined in Section 31.5.

Since \( A^{-1} \) is symmetric positive definite and
\[ L(x, \lambda) = \frac{1}{2} x^\top A^{-1} x - (b - B\lambda)^\top x - \lambda^\top f, \]
by Proposition 23.2 the global minimum (with respect to \( x \)) of \( L(x, \lambda) \) is obtained for the solution \( x \) of
\[ A^{-1} x = b - B\lambda, \]
that is, when
\[ x = A(b - B\lambda), \]
and the minimum of \( L(x, \lambda) \) is
\[ \min_x L(x, \lambda) = \frac{1}{2} (B\lambda - b)^\top A(B\lambda - b) - \lambda^\top f. \]

Letting
\[ G(\lambda) = \frac{1}{2} (B\lambda - b)^\top A(B\lambda - b) + \lambda^\top f, \]
we will show in Proposition 23.3 that the solution of the constrained minimization of \( Q(x) \) subject to \( B^\top x = f \) is equivalent to the unconstrained maximization of \( -G(\lambda) \). This is a special case of the duality discussed in Section 31.5.

Of course, since we minimized \( L(x, \lambda) \) with respect to \( x \), we have
\[ L(x, \lambda) \geq -G(\lambda) \]
for all \( x \) and all \( \lambda \). However, when the constraint \( B^\top x = f \) holds, \( L(x, \lambda) = Q(x) \), and thus for any admissible \( x \), which means that \( B^\top x = f \), we have

\[
\min_x Q(x) \geq \max_\lambda -G(\lambda).
\]

In order to prove that the unique minimum of the constrained problem \( Q(x) \) subject to \( B^\top x = f \) is the unique maximum of \(-G(\lambda)\), we compute \( Q(x) + G(\lambda) \).

**Proposition 6.3.** The quadratic constrained minimization problem of Definition 23.3 has a unique solution \((x, \lambda)\) given by the system

\[
\begin{pmatrix}
A^{-1} & B \\
B^\top & 0
\end{pmatrix}
\begin{pmatrix}
x \\
\lambda
\end{pmatrix} =
\begin{pmatrix}
b \\
f
\end{pmatrix}.
\]

Furthermore, the component \( \lambda \) of the above solution is the unique value for which \(-G(\lambda)\) is maximum.

**Proof.** As we suggested earlier, let us compute \( Q(x) + G(\lambda) \), assuming that the constraint \( B^\top x = f \) holds. Eliminating \( f \), since \( b^\top x = x^\top b \) and \( \lambda^\top B^\top x = x^\top B\lambda \), we get

\[
Q(x) + G(\lambda) = \frac{1}{2} x^\top A^{-1} x - b^\top x + \frac{1}{2} (B\lambda - b)^\top A(B\lambda - b) + \lambda^\top f
\]

\[
= \frac{1}{2} (A^{-1} x + B\lambda - b)^\top A(A^{-1} x + B\lambda - b).
\]

Since \( A \) is positive definite, the last expression is nonnegative. In fact, it is null iff

\[
A^{-1} x + B\lambda - b = 0,
\]

that is,

\[
A^{-1} x + B\lambda = b.
\]

But then the unique constrained minimum of \( Q(x) \) subject to \( B^\top x = f \) is equal to the unique maximum of \(-G(\lambda)\) exactly when \( B^\top x = f \) and \( A^{-1} x + B\lambda = b \), which proves the proposition. \( \square \)

We can confirm that the maximum of \(-G(\lambda)\), or equivalently the minimum of

\[
G(\lambda) = \frac{1}{2} (B\lambda - b)^\top A(B\lambda - b) + \lambda^\top f,
\]

corresponds to value of \( \lambda \) obtained by solving the system

\[
\begin{pmatrix}
A^{-1} & B \\
B^\top & 0
\end{pmatrix}
\begin{pmatrix}
x \\
\lambda
\end{pmatrix} =
\begin{pmatrix}
b \\
f
\end{pmatrix}.
\]

Indeed, since

\[
G(\lambda) = \frac{1}{2} \lambda^\top B^\top AB\lambda - \lambda^\top B^\top Ab + \lambda^\top f + \frac{1}{2} b^\top b,
\]
and $B^\top AB$ is symmetric positive definite, by Proposition 23.2, the global minimum of $G(\lambda)$ is obtained when

$$B^\top AB\lambda - B^\top Ab + f = 0,$$

that is, $\lambda = (B^\top AB)^{-1}(B^\top Ab - f)$, as we found earlier.

Remarks:

1. There is a form of duality going on in this situation. The constrained minimization of $Q(x)$ subject to $B^\top x = f$ is called the **primal problem**, and the unconstrained maximization of $-G(\lambda)$ is called the **dual problem**. Duality is the fact stated slightly loosely as

$$\min_x Q(x) = \max_\lambda -G(\lambda).$$

A general treatment of duality in constrained minimization problems is given in Section 31.5.

Recalling that $e = b - B\lambda$, since

$$G(\lambda) = \frac{1}{2}(B\lambda - b)^\top A(B\lambda - b) + \lambda^\top f,$$

we can also write

$$G(\lambda) = \frac{1}{2}e^\top Ae + \lambda^\top f.$$ 

This expression often represents the total potential energy of a system. Again, the optimal solution is the one that minimizes the potential energy (and thus maximizes $-G(\lambda)$).

2. It is immediately verified that the equations of Proposition 23.3 are equivalent to the equations stating that the partial derivatives of the Lagrangian $L(x, \lambda)$ are null:

$$\frac{\partial L}{\partial x_i} = 0, \quad i = 1, \ldots, m,$$

$$\frac{\partial L}{\partial \lambda_j} = 0, \quad j = 1, \ldots, n.$$ 

Thus, the constrained minimum of $Q(x)$ subject to $B^\top x = f$ is an extremum of the Lagrangian $L(x, \lambda)$. As we showed in Proposition 23.3, this extremum corresponds to simultaneously minimizing $L(x, \lambda)$ with respect to $x$ and maximizing $L(x, \lambda)$ with respect to $\lambda$. Geometrically, such a point is a **saddle point** for $L(x, \lambda)$. Saddle points are discussed in Section 31.5.

3. The Lagrange multipliers sometimes have a natural physical meaning. For example, in the spring-mass system they correspond to node displacements. In some general sense, Lagrange multipliers are correction terms needed to satisfy equilibrium equations and the price paid for the constraints. For more details, see Strang [102].
Going back to the constrained minimization of \( Q(x_1, x_2) = \frac{1}{2}(x_1^2 + x_2^2) \) subject to
\[
2x_1 - x_2 = 5,
\]
the Lagrangian is
\[
L(x_1, x_2, \lambda) = \frac{1}{2}(x_1^2 + x_2^2) + \lambda(2x_1 - x_2 - 5),
\]
and the equations stating that the Lagrangian has a saddle point are
\[
\begin{align*}
x_1 + 2\lambda &= 0, \\
x_2 - \lambda &= 0, \\
2x_1 - x_2 - 5 &= 0.
\end{align*}
\]
We obtain the solution \((x_1, x_2, \lambda) = (2, -1, -1)\).

The use of Lagrange multipliers in optimization and variational problems is discussed extensively in Chapter 31.

Least squares methods and Lagrange multipliers are used to tackle many problems in computer graphics and computer vision; see Trucco and Verri [107], Metaxas [74], Jain, Katsuri, and Schunck [58], Faugeras [40], and Foley, van Dam, Feiner, and Hughes [41].

### 6.2 Quadratic Optimization: The General Case

In this section we complete the study initiated in Section 23.1 and give necessary and sufficient conditions for the quadratic function \( \frac{1}{2}x^\top Ax - x^\top b \) to have a global minimum. We begin with the following simple fact:

**Proposition 6.4.** If \( A \) is an invertible symmetric matrix, then the function
\[
f(x) = \frac{1}{2}x^\top Ax - x^\top b
\]
has a minimum value iff \( A \succeq 0 \), in which case this optimal value is obtained for a unique value of \( x \), namely \( x^* = A^{-1}b \), and with
\[
f(A^{-1}b) = -\frac{1}{2}b^\top A^{-1}b.
\]

**Proof.** Observe that
\[
\frac{1}{2}(x - A^{-1}b)^\top A(x - A^{-1}b) = \frac{1}{2}x^\top Ax - x^\top b + \frac{1}{2}b^\top A^{-1}b.
\]
Thus,
\[
f(x) = \frac{1}{2}x^\top Ax - x^\top b = \frac{1}{2}(x - A^{-1}b)^\top A(x - A^{-1}b) - \frac{1}{2}b^\top A^{-1}b.
\]
If $A$ has some negative eigenvalue, say $-\lambda$ (with $\lambda > 0$), if we pick any eigenvector $u$ of $A$ associated with $\lambda$, then for any $\alpha \in \mathbb{R}$ with $\alpha \neq 0$, if we let $x = \alpha u + A^{-1}b$, then since $Au = -\lambda u$, we get
\[
 f(x) = \frac{1}{2} (x - A^{-1}b)^\top A(x - A^{-1}b) - \frac{1}{2} b^\top A^{-1}b \\
 = \frac{1}{2} \alpha u^\top A\alpha u - \frac{1}{2} b^\top A^{-1}b \\
 = -\frac{1}{2} \alpha^2 \lambda \|u\|_2^2 - \frac{1}{2} b^\top A^{-1}b,
\]
and since $\alpha$ can be made as large as we want and $\lambda > 0$, we see that $f$ has no minimum. Consequently, in order for $f$ to have a minimum, we must have $A \succeq 0$. If $A \succeq 0$, since $A$ is invertible, it is positive definite, so $(x - A^{-1}b)^\top A(x - A^{-1}b) > 0$ iff $x - A^{-1}b \neq 0$, and it is clear that the minimum value of $f$ is achieved when $x - A^{-1}b = 0$, that is, $x = A^{-1}b$. \[\square\]

Let us now consider the case of an arbitrary symmetric matrix $A$.

**Proposition 6.5.** If $A$ is a $n \times n$ symmetric matrix, then the function
\[
 f(x) = \frac{1}{2} x^\top Ax - x^\top b
\]
has a minimum value iff $A \succeq 0$ and $(I - AA^+)b = 0$, in which case this minimum value is
\[
 p^* = -\frac{1}{2} b^\top A^+ b.
\]
Furthermore, if $A$ is diagonalized as $A = U^\top \Sigma U$ (with $U$ orthogonal), then the optimal value is achieved by all $x \in \mathbb{R}^n$ of the form
\[
 x = A^+ b + U^\top \begin{pmatrix} 0 \\ z \end{pmatrix},
\]
for any $z \in \mathbb{R}^{n-r}$, where $r$ is the rank of $A$.

**Proof.** The case that $A$ is invertible is taken care of by Proposition 23.4, so we may assume that $A$ is singular. If $A$ has rank $r < n$, then we can diagonalize $A$ as
\[
 A = U^\top \begin{pmatrix} \Sigma_r & 0 \\ 0 & 0 \end{pmatrix} U,
\]
where $U$ is an orthogonal matrix and where $\Sigma_r$ is an $r \times r$ diagonal invertible matrix. Then we have
\[
 f(x) = \frac{1}{2} x^\top U^\top \begin{pmatrix} \Sigma_r & 0 \\ 0 & 0 \end{pmatrix} U x - x^\top U^\top Ub \\
 = \frac{1}{2} (Ux)^\top \begin{pmatrix} \Sigma_r & 0 \\ 0 & 0 \end{pmatrix} U x - (Ux)^\top Ub.
\]
If we write

\[ Ux = \begin{pmatrix} y \\ z \end{pmatrix} \quad \text{and} \quad Ub = \begin{pmatrix} c \\ d \end{pmatrix}, \]

with \( y, c \in \mathbb{R}^r \) and \( z, d \in \mathbb{R}^{n-r} \), we get

\[
\begin{align*}
    f(x) &= \frac{1}{2} (Ux)\top \left( \begin{array}{cc} \Sigma_r & 0 \\ 0 & 0 \end{array} \right) Ux - (Ux)\top Ub \\
         &= \frac{1}{2} (y\top z\top) \left( \begin{array}{cc} \Sigma_r & 0 \\ 0 & 0 \end{array} \right) \left( \begin{array}{c} y \\ z \end{array} \right) - (y\top z\top) \left( \begin{array}{c} c \\ d \end{array} \right) \\
         &= \frac{1}{2} y\top y\top \Sigma_r y - y\top c - z\top d.
\end{align*}
\]

For \( y = 0 \), we get

\[ f(x) = -z\top d, \]

so if \( d \neq 0 \), the function \( f \) has no minimum. Therefore, if \( f \) has a minimum, then \( d = 0 \). However, \( d = 0 \) means that

\[
Ub = \begin{pmatrix} c \\ 0 \end{pmatrix},
\]

and we know from Proposition 17.5 (Vol. I) that \( b \) is in the range of \( A \) (here, \( U \) is \( V\top \)), which is equivalent to \( (I - AA\top)b = 0 \). If \( d = 0 \), then

\[
f(x) = \frac{1}{2} y\top \Sigma_r y - y\top c,
\]

and since \( \Sigma_r \) is invertible, by Proposition 23.4, the function \( f \) has a minimum iff \( \Sigma_r \succeq 0 \), which is equivalent to \( A \succeq 0 \).

Therefore, we have proved that if \( f \) has a minimum, then \( (I - AA\top)b = 0 \) and \( A \succeq 0 \). Conversely, if \( (I - AA\top)b = 0 \) and \( A \succeq 0 \), what we just did proves that \( f \) does have a minimum.

When the above conditions hold, since

\[
A = U\top \left( \begin{array}{cc} \Sigma_r & 0 \\ 0 & 0 \end{array} \right) U
\]

is positive semidefinite, the pseudo-inverse \( A\top \) of \( A \) is given by

\[
A\top = U\top \left( \begin{array}{cc} \Sigma_r^{-1} & 0 \\ 0 & 0 \end{array} \right) U,
\]

and by Proposition 23.4 the minimum is achieved if \( y = \Sigma_r^{-1} c \), \( z = 0 \) and \( d = 0 \), that is, for \( x^* \) given by

\[
Ux^* = \begin{pmatrix} \Sigma_r^{-1} c \\ 0 \end{pmatrix} \quad \text{and} \quad Ub = \begin{pmatrix} c \\ 0 \end{pmatrix},
\]
from which we deduce that
\[ x^* = U^T \begin{pmatrix} \Sigma_r^{-1} c \\ 0 \end{pmatrix} = U^T \begin{pmatrix} \Sigma_r^{-1} & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} c \\ 0 \end{pmatrix} = U^T \begin{pmatrix} \Sigma_r^{-1} & 0 \\ 0 & 0 \end{pmatrix} U b = A^+ b \]
and the minimum value of \( f \) is
\[ f(x^*) = -\frac{1}{2} b^T A^+ b. \]
For any \( x \in \mathbb{R}^n \) of the form
\[ x = A^+ b + U^T \begin{pmatrix} 0 \\ z \end{pmatrix}, \]
for any \( z \in \mathbb{R}^{n-r} \), we have
\[
\begin{align*}
  f(x) &= \frac{1}{2} \left( A^+ b + U^T \begin{pmatrix} 0 \\ z \end{pmatrix} \right)^T A \left( A^+ b + U^T \begin{pmatrix} 0 \\ z \end{pmatrix} \right) - \left( A^+ b + U^T \begin{pmatrix} 0 \\ z \end{pmatrix} \right)^T b \\
  &= \frac{1}{2} (A^+ b)^T A A^+ b + (0 z^T) U A A^+ b + \frac{1}{2} (0 z^T) U A U^T \begin{pmatrix} 0 \\ z \end{pmatrix} - (A^+ b)^T b - (0 z^T) U b \\
  &= -\frac{1}{2} b^T A^+ b + (0 z^T) U A A^+ b + \frac{1}{2} (0 z^T) U A U^T \begin{pmatrix} 0 \\ z \end{pmatrix} - (0 z^T) U b.
\end{align*}
\]
We have
\[
\begin{align*}
  (0 z^T) U A A^+ b &= (0 z^T) U U^T \begin{pmatrix} \Sigma_r & 0 \\ 0 & 0 \end{pmatrix} U U^T \begin{pmatrix} \Sigma_r^{-1} & 0 \\ 0 & 0 \end{pmatrix} U b \\
  &= (0 z^T) \begin{pmatrix} I_r & 0 \\ 0 & 0 \end{pmatrix} U b = 0,
\end{align*}
\]
\[
\begin{align*}
  (0 z^T) U A U^T \begin{pmatrix} 0 \\ z \end{pmatrix} &= (0 z^T) U U^T \begin{pmatrix} \Sigma_r & 0 \\ 0 & 0 \end{pmatrix} U U^T \begin{pmatrix} 0 \\ z \end{pmatrix} \\
  &= (0 z^T) \begin{pmatrix} \Sigma_r & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ z \end{pmatrix} = 0,
\end{align*}
\]
and
\[ (0 z^T) U b = (0 z^T) \begin{pmatrix} c \\ 0 \end{pmatrix} = 0, \]
because \( (I - A A^+) b = 0 \), that is,
\[
\begin{align*}
  \left( \begin{pmatrix} I_r & 0 \\ 0 & I_{n-r} \end{pmatrix} - U^T \begin{pmatrix} \Sigma_r & 0 \\ 0 & 0 \end{pmatrix} U U^T \begin{pmatrix} \Sigma_r^{-1} & 0 \\ 0 & 0 \end{pmatrix} U \right) b &= \left( \begin{pmatrix} I_r & 0 \\ 0 & I_{n-r} \end{pmatrix} - U^T \begin{pmatrix} I_r & 0 \\ 0 & 0 \end{pmatrix} U \right) b \\
  &= U^T \begin{pmatrix} 0 & 0 \\ 0 & I_{n-r} \end{pmatrix} U b = 0,
\end{align*}
\]
so if
\[ U b = \begin{pmatrix} c \\ d \end{pmatrix}, \]
then \( d = 0 \). Therefore, \( f(x) = -\frac{1}{2} b^T A^+ b \). \qed
The problem of minimizing the function
\[ f(x) = \frac{1}{2} x^\top A x - x^\top b \]
in the case where we add either linear constraints of the form \( C^\top x = 0 \) or affine constraints of the form \( C^\top x = t \) (where \( t \in \mathbb{R}^m \) and \( t \neq 0 \)) where \( C \) is an \( n \times m \) matrix can be reduced to the unconstrained case using a \( QR \)-decomposition of \( C \). Let us show how to do this for linear constraints of the form \( C^\top x = 0 \).

If we use a \( QR \) decomposition of \( C \), by permuting the columns of \( C \) to make sure that the first \( r \) columns of \( C \) are linearly independent (where \( r = \text{rank}(C) \)), we may assume that
\[
C = Q^\top \begin{pmatrix} R & S \\ 0 & 0 \end{pmatrix} \Pi,
\]
where \( Q \) is an \( n \times n \) orthogonal matrix, \( R \) is an \( r \times r \) invertible upper triangular matrix, \( S \) is an \( r \times (m - r) \) matrix, and \( \Pi \) is a permutation matrix (\( C \) has rank \( r \)). Then if we let
\[
x = Q^\top \begin{pmatrix} y \\ z \end{pmatrix},
\]
where \( y \in \mathbb{R}^r \) and \( z \in \mathbb{R}^{n-r} \), then \( C^\top x = 0 \) becomes
\[
C^\top x = \Pi^\top \begin{pmatrix} R^\top \\ S^\top \end{pmatrix} 0 \) Qx = \Pi^\top \begin{pmatrix} R^\top & 0 \\ S^\top & 0 \end{pmatrix} \begin{pmatrix} y \\ z \end{pmatrix} = 0,
\]
which implies \( y = 0 \), and every solution of \( C^\top x = 0 \) is of the form
\[
x = Q^\top \begin{pmatrix} 0 \\ z \end{pmatrix}.
\]

Our original problem becomes
\[
\begin{align*}
\text{minimize} & \quad \frac{1}{2} (y^\top z^\top)Q A Q^\top \begin{pmatrix} y \\ z \end{pmatrix} + (y^\top z^\top)Qb \\
\text{subject to} & \quad y = 0, \; y \in \mathbb{R}^r, \; z \in \mathbb{R}^{n-r}.
\end{align*}
\]
Thus, the constraint \( C^\top x = 0 \) has been simplified to \( y = 0 \), and if we write
\[
Q A Q^\top = \begin{pmatrix} G_{11} & G_{12} \\ G_{21} & G_{22} \end{pmatrix},
\]
where \( G_{11} \) is an \( r \times r \) matrix and \( G_{22} \) is an \( (n - r) \times (n - r) \) matrix, and
\[
Qb = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}, \quad b_1 \in \mathbb{R}^r, \; b_2 \in \mathbb{R}^{n-r},
\]
our problem becomes
\[
\text{minimize } \frac{1}{2} z^\top G_{22} z + z^\top b_2, \quad z \in \mathbb{R}^{n-r},
\]
the problem solved in Proposition 23.5.

Constraints of the form \( C^\top x = t \) (where \( t \neq 0 \)) can be handled in a similar fashion. In this case, we may assume that \( C \) is an \( n \times m \) matrix with full rank (so that \( m \leq n \)) and \( t \in \mathbb{R}^m \). Then we use a QR-decomposition of the form
\[
C = P \begin{pmatrix} R \\ 0 \end{pmatrix},
\]
where \( P \) is an orthogonal \( n \times n \) matrix and \( R \) is an \( m \times m \) invertible upper triangular matrix. If we write
\[
x = P \begin{pmatrix} y \\ z \end{pmatrix},
\]
where \( y \in \mathbb{R}^m \) and \( z \in \mathbb{R}^{n-m} \), the equation \( C^\top x = t \) becomes
\[
(R^\top 0) P^\top x = t,
\]
that is,
\[
(R^\top 0) \begin{pmatrix} y \\ z \end{pmatrix} = t,
\]
which yields
\[
R^\top y = t.
\]
Since \( R \) is invertible, we get \( y = (R^\top)^{-1} t \), and then it is easy to see that our original problem reduces to an unconstrained problem in terms of the matrix \( P^\top A P \); the details are left as an exercise.

### 6.3 Maximizing a Quadratic Function on the Unit Sphere

In this section we discuss various quadratic optimization problems mostly arising from computer vision (image segmentation and contour grouping). These problems can be reduced to the following basic optimization problem: Given an \( n \times n \) real symmetric matrix \( A \)
\[
\begin{align*}
\text{maximize} & \quad x^\top A x \\
\text{subject to} & \quad x^\top x = 1, \quad x \in \mathbb{R}^n.
\end{align*}
\]

In view of Proposition 17.10 (Vol. I), the maximum value of \( x^\top A x \) on the unit sphere is equal to the largest eigenvalue \( \lambda_1 \) of the matrix \( A \), and it is achieved for any unit eigenvector \( u_1 \) associated with \( \lambda_1 \).
A variant of the above problem often encountered in computer vision consists in mini-
mizing $x^\top Ax$ on the ellipsoid given by an equation of the form

$$x^\top Bx = 1,$$

where $B$ is a symmetric positive definite matrix. Since $B$ is positive definite, it can be
diagonalized as

$$B = QDQ^\top,$$

where $Q$ is an orthogonal matrix and $D$ is a diagonal matrix,

$$D = \text{diag}(d_1, \ldots, d_n),$$

with $d_i > 0$, for $i = 1, \ldots, n$. If we define the matrices $B^{1/2}$ and $B^{-1/2}$ by

$$B^{1/2} = Q \text{diag} \left( \sqrt{d_1}, \ldots, \sqrt{d_n} \right) Q^\top$$

and

$$B^{-1/2} = Q \text{diag} \left( 1/\sqrt{d_1}, \ldots, 1/\sqrt{d_n} \right) Q^\top,$$

it is clear that these matrices are symmetric, that $B^{-1/2}BB^{-1/2} = I$, and that $B^{1/2}$ and
$B^{-1/2}$ are mutual inverses. Then, if we make the change of variable

$$x = B^{-1/2}y,$$

the equation $x^\top Bx = 1$ becomes $y^\top y = 1$, and the optimization problem

$$\begin{align*}
\text{maximize} & \quad x^\top Ax \\
\text{subject to} & \quad x^\top Bx = 1, \ x \in \mathbb{R}^n,
\end{align*}$$

is equivalent to the problem

$$\begin{align*}
\text{maximize} & \quad y^\top B^{-1/2}AB^{-1/2}y \\
\text{subject to} & \quad y^\top y = 1, \ y \in \mathbb{R}^n,
\end{align*}$$

where $y = B^{1/2}x$ and where $B^{-1/2}AB^{-1/2}$ is symmetric.

The complex version of our basic optimization problem in which $A$ is a Hermitian matrix
also arises in computer vision. Namely, given an $n \times n$ complex Hermitian matrix $A$,

$$\begin{align*}
\text{maximize} & \quad x^* A x \\
\text{subject to} & \quad x^* x = 1, \ x \in \mathbb{C}^n.
\end{align*}$$

Again by Proposition 17.10 (Vol. I), the maximum value of $x^* A x$ on the unit sphere is
equal to the largest eigenvalue $\lambda_1$ of the matrix $A$ and it is achieved for any unit eigenvector
$u_1$ associated with $\lambda_1$. 
Remark: It is worth pointing out that if $A$ is a skew-Hermitian matrix, that is, if $A^* = -A$, then $x^*Ax$ is pure imaginary or zero.

Indeed, since $z = x^*Ax$ is a scalar, we have $z^* = \bar{z}$ (the conjugate of $z$), so we have

$$\bar{x^*Ax} = (x^*Ax)^* = x^*A^*x = -x^*Ax,$$

so $x^*Ax + x^*Ax = 2\text{Re}(x^*Ax) = 0$, which means that $x^*Ax$ is pure imaginary or zero.

In particular, if $A$ is a real matrix and if $A$ is skew-symmetric, then

$$x^\top Ax = 0.$$

Thus, for any real matrix (symmetric or not),

$$x^\top Ax = x^\top H(A)x,$$

where $H(A) = (A + A^\top)/2$, the symmetric part of $A$.

There are situations in which it is necessary to add linear constraints to the problem of maximizing a quadratic function on the sphere. This problem was completely solved by Golub [48] (1973). The problem is the following: Given an $n \times n$ real symmetric matrix $A$ and an $n \times p$ matrix $C$,

$$\begin{align*}
\text{minimize} & \quad x^\top Ax \\
\text{subject to} & \quad x^\top x = 1, \quad C^\top x = 0, \quad x \in \mathbb{R}^n.
\end{align*}$$

As in Section 23.2, Golub shows that the linear constraint $C^\top x = 0$ can be eliminated as follows: If we use a QR decomposition of $C$, by permuting the columns, we may assume that

$$C = Q^\top \begin{pmatrix} R & S \\ 0 & 0 \end{pmatrix} \Pi,$$

where $Q$ is an orthogonal $n \times n$ matrix, $R$ is an $r \times r$ invertible upper triangular matrix, and $S$ is an $r \times (p - r)$ matrix (assuming $C$ has rank $r$). Then if we let

$$x = Q^\top \begin{pmatrix} y \\ z \end{pmatrix},$$

where $y \in \mathbb{R}^r$ and $z \in \mathbb{R}^{n-r}$, then $C^\top x = 0$ becomes

$$\Pi^\top \begin{pmatrix} R^\top & 0 \\ S^\top & 0 \end{pmatrix} Qx = \Pi^\top \begin{pmatrix} R^\top & 0 \\ S^\top & 0 \end{pmatrix} \begin{pmatrix} y \\ z \end{pmatrix} = 0,$$

which implies $y = 0$, and every solution of $C^\top x = 0$ is of the form

$$x = Q^\top \begin{pmatrix} 0 \\ z \end{pmatrix}.$$
Our original problem becomes

$$\begin{align*}
\text{minimize} & \quad (y^\top z^\top)QAQ^\top \begin{pmatrix} y \\ z \end{pmatrix} \\
\text{subject to} & \quad z^\top z = 1, \ z \in \mathbb{R}^{n-r}, \\
& \quad y = 0, \ y \in \mathbb{R}^r.
\end{align*}$$

Thus, the constraint $C^\top x = 0$ has been simplified to $y = 0$, and if we write

$$QAQ^\top = \begin{pmatrix} G_{11} & G_{12} \\
G_{12}^\top & G_{22} \end{pmatrix},$$

our problem becomes

$$\begin{align*}
\text{minimize} & \quad z^\top G_{22} z \\
\text{subject to} & \quad z^\top z = 1, \ z \in \mathbb{R}^{n-r},
\end{align*}$$
a standard eigenvalue problem.

**Remark:** There is a way of finding the eigenvalues of $G_{22}$ which does not require the $QR$-factorization of $C$. Observe that if we let

$$J = \begin{pmatrix} 0 & 0 \\
0 & I_{n-r} \end{pmatrix},$$

then

$$JQAQ^\top J = \begin{pmatrix} 0 & 0 \\
0 & G_{22} \end{pmatrix},$$

and if we set

$$P = Q^\top JQ,$$

then

$$PAP = Q^\top JQAQ^\top JQ.$$

Now, $Q^\top JQAQ^\top JQ$ and $JQAQ^\top J$ have the same eigenvalues, so $PAP$ and $JQAQ^\top J$ also have the same eigenvalues. It follows that the solutions of our optimization problem are among the eigenvalues of $K = PAP$, and at least $r$ of those are $0$. Using the fact that $CC^+$ is the projection onto the range of $C$, where $C^+$ is the pseudo-inverse of $C$, it can also be shown that

$$P = I - CC^+,$$

the projection onto the kernel of $C^\top$. So $P$ can be computed directly in terms of $C$. In particular, when $n \geq p$ and $C$ has full rank (the columns of $C$ are linearly independent), then we know that $C^+ = (C^\top C)^{-1}C^\top$ and

$$P = I - C(C^\top C)^{-1}C^\top.$$
This fact is used by Cour and Shi [31] and implicitly by Yu and Shi [113].

The problem of adding affine constraints of the form \( N^\top x = t \), where \( t \neq 0 \), also comes up in practice. At first glance, this problem may not seem harder than the linear problem in which \( t = 0 \), but it is. This problem was extensively studied in a paper by Gander, Golub, and von Matt [46] (1989).

Gander, Golub, and von Matt consider the following problem: Given an \((n+m) \times (n+m)\) real symmetric matrix \( A \) (with \( n > 0 \)), an \((n+m) \times m\) matrix \( N \) with full rank, and a nonzero vector \( t \in \mathbb{R}^m \) with \( \|(N^\top)^+t\| < 1 \) (where \((N^\top)^+\) denotes the pseudo-inverse of \( N^\top \)),

\[
\begin{align*}
\text{minimize} & \quad x^\top Ax \\
\text{subject to} & \quad x^\top x = 1, \quad N^\top x = t, \quad x \in \mathbb{R}^{n+m}.
\end{align*}
\]

The condition \( \|(N^\top)^+t\| < 1 \) ensures that the problem has a solution and is not trivial. The authors begin by proving that the affine constraint \( N^\top x = t \) can be eliminated. One way to do so is to use a QR decomposition of \( N \). If

\[
N = P \begin{pmatrix} R \\ 0 \end{pmatrix},
\]

where \( P \) is an orthogonal \((n+m) \times (n+m)\) matrix and \( R \) is an \( m \times m \) invertible upper triangular matrix, then if we observe that

\[
\begin{align*}
x^\top Ax &= x^\top PP^\top APP^\top x, \\
N^\top x &= (R^\top 0)P^\top x = t, \\
x^\top x &= x^\top PP^\top x = 1,
\end{align*}
\]

and if we write

\[
P^\top AP = \begin{pmatrix} B & \Gamma^\top \\ \Gamma & C \end{pmatrix},
\]

where \( B \) is an \( m \times m \) symmetric matrix, \( C \) is an \( n \times n \) symmetric matrix, \( \Gamma \) is an \( m \times n \) matrix, and

\[
P^\top x = \begin{pmatrix} y \\ z \end{pmatrix},
\]

with \( y \in \mathbb{R}^m \) and \( z \in \mathbb{R}^n \), then we get

\[
\begin{align*}
x^\top Ax &= y^\top By + 2z^\top \Gamma y + z^\top Cz, \\
R^\top y &= t, \\
y^\top y + z^\top z &= 1.
\end{align*}
\]

Thus

\[
y = (R^\top)^{-1} t,
\]
and if we write
\[ s^2 = 1 - y^\top y > 0 \]
and
\[ b = \Gamma y, \]
we get the simplified problem
\[
\begin{align*}
\text{minimize} & \quad z^\top Cz + 2z^\top b \\
\text{subject to} & \quad z^\top z = s^2, \quad z \in \mathbb{R}^m.
\end{align*}
\]
Unfortunately, if \( b \neq 0 \), Proposition 17.10 (Vol. I) is no longer applicable. It is still possible to find the minimum of the function \( z^\top Cz + 2z^\top b \) using Lagrange multipliers, but such a solution is too involved to be presented here. Interested readers will find a thorough discussion in Gander, Golub, and von Matt [46].

### 6.4 Summary

The main concepts and results of this chapter are listed below:

- Quadratic optimization problems; \textit{quadratic functions}.
- Symmetric \textit{positive definite} and \textit{positive semidefinite} matrices.
- The \textit{positive semidefinite cone ordering}.
- Existence of a global minimum when \( A \) is symmetric positive definite.
- Constrained quadratic optimization problems.
- \textit{Lagrange multipliers; Lagrangian}.
- \textit{Primal} and \textit{dual} problems.
- Quadratic optimization problems: the case of a symmetric invertible matrix \( A \).
- Quadratic optimization problems: the general case of a symmetric matrix \( A \).
- Adding linear constraints of the form \( C^\top x = 0 \).
- Adding affine constraints of the form \( C^\top x = t \), with \( t \neq 0 \).
- Maximizing a quadratic function over the unit sphere.
- Maximizing a quadratic function over an ellipsoid.
- Maximizing a Hermitian quadratic form.
- Adding linear constraints of the form \( C^\top x = 0 \).
- Adding affine constraints of the form \( N^\top x = t \), with \( t \neq 0 \).
Chapter 7

Schur Complements and Applications

7.1 Schur Complements

Schur complements arise naturally in the process of inverting block matrices of the form

\[ M = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \]

and in characterizing when symmetric versions of these matrices are positive definite or positive semidefinite. These characterizations come up in various quadratic optimization problems; see Boyd and Vandenberghe [22], especially Appendix B. In the most general case, pseudo-inverses are also needed.

In this chapter we introduce Schur complements and describe several interesting ways in which they are used. Along the way we provide some details and proofs of some results from Appendix A.5 (especially Section A.5.5) of Boyd and Vandenberghe [22].

Let \( M \) be an \( n \times n \) matrix written as a \( 2 \times 2 \) block matrix

\[ M = \begin{pmatrix} A & B \\ C & D \end{pmatrix}, \]

where \( A \) is a \( p \times p \) matrix and \( D \) is a \( q \times q \) matrix, with \( n = p + q \) (so \( B \) is a \( p \times q \) matrix and \( C \) is a \( q \times p \) matrix). We can try to solve the linear system

\[ \begin{pmatrix} A & B \\ C & D \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} c \\ d \end{pmatrix}, \]

that is,

\[ Ax + By = c, \]
\[ Cx + Dy = d, \]

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by mimicking Gaussian elimination. If we assume that $D$ is invertible, then we first solve for $y$, getting

$$y = D^{-1}(d - Cx),$$

and after substituting this expression for $y$ in the first equation, we get

$$Ax + B(D^{-1}(d - Cx)) = c,$$

that is,

$$(A - BD^{-1}C)x = c - BD^{-1}d.$$  

If the matrix $A - BD^{-1}C$ is invertible, then we obtain the solution to our system

$$x = (A - BD^{-1}C)^{-1}(c - BD^{-1}d),$$
$$y = D^{-1}(d - C(A - BD^{-1}C)^{-1}(c - BD^{-1}d)).$$

If $A$ is invertible, then by eliminating $x$ first using the first equation, we obtain analogous formulas involving the matrix $D - CA^{-1}B$. The above formulas suggest that the matrices $A - BD^{-1}C$ and $D - CA^{-1}B$ play a special role and suggest the following definition:

**Definition 7.1.** Given any $n \times n$ block matrix of the form

$$M = \begin{pmatrix} A & B \\ C & D \end{pmatrix},$$

where $A$ is a $p \times p$ matrix and $D$ is a $q \times q$ matrix, with $n = p + q$ (so $B$ is a $p \times q$ matrix and $C$ is a $q \times p$ matrix), if $D$ is invertible, then the matrix $A - BD^{-1}C$ is called the Schur complement of $D$ in $M$. If $A$ is invertible, then the matrix $D - CA^{-1}B$ is called the Schur complement of $A$ in $M$.

The above equations written as

$$x = (A - BD^{-1}C)^{-1}c - (A - BD^{-1}C)^{-1}BD^{-1}d,$$
$$y = -D^{-1}C(A - BD^{-1}C)^{-1}c + (D^{-1} + D^{-1}C(A - BD^{-1}C)^{-1}BD^{-1})d,$$

yield a formula for the inverse of $M$ in terms of the Schur complement of $D$ in $M$, namely

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix}^{-1} = \begin{pmatrix} (A - BD^{-1}C)^{-1} & -(A - BD^{-1}C)^{-1}BD^{-1} \\ -D^{-1}C(A - BD^{-1}C)^{-1} & D^{-1} + D^{-1}C(A - BD^{-1}C)^{-1}BD^{-1} \end{pmatrix}.$$ 

A moment of reflection reveals that

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix}^{-1} = \begin{pmatrix} (A - BD^{-1}C)^{-1} & 0 \\ -D^{-1}C(A - BD^{-1}C)^{-1} & D^{-1} \end{pmatrix},$$

and then

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix}^{-1} = \begin{pmatrix} I & 0 \\ -D^{-1}C & I \end{pmatrix} \begin{pmatrix} (A - BD^{-1}C)^{-1} & 0 \\ 0 & D^{-1} \end{pmatrix} \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix}.$$ 

By taking inverses, we obtain the following result.
Proposition 7.1. If the matrix $D$ is invertible, then
\[
\begin{pmatrix} A & B \\ C & D \end{pmatrix} = \begin{pmatrix} I & BD^{-1} \\ 0 & I \end{pmatrix} \begin{pmatrix} A - BD^{-1}C & 0 \\ 0 & D \end{pmatrix} \begin{pmatrix} I & 0 \\ D^{-1}C & I \end{pmatrix}.
\]

The above expression can be checked directly and has the advantage of requiring only the invertibility of $D$.

Remark: If $A$ is invertible, then we can use the Schur complement $D - CA^{-1}B$ of $A$ to obtain the following factorization of $M$:
\[
\begin{pmatrix} A & B \\ C & D \end{pmatrix} = \begin{pmatrix} I & 0 \\ CA^{-1} & I \end{pmatrix} \begin{pmatrix} A & 0 \\ 0 & D - CA^{-1}B \end{pmatrix} \begin{pmatrix} I & A^{-1}B \\ 0 & I \end{pmatrix}.
\]

If $D - CA^{-1}B$ is invertible, we can invert all three matrices above, and we get another formula for the inverse of $M$ in terms of $(D - CA^{-1}B)$, namely,
\[
\begin{pmatrix} A & B \\ C & D \end{pmatrix}^{-1} = \begin{pmatrix} A^{-1} + A^{-1}B(D - CA^{-1}B)^{-1}CA^{-1} & -A^{-1}B(D - CA^{-1}B)^{-1} \\ -(D - CA^{-1}B)^{-1}CA^{-1} & (D - CA^{-1}B)^{-1} \end{pmatrix}.
\]

If $A, D$ and both Schur complements $A - BD^{-1}C$ and $D - CA^{-1}B$ are all invertible, by comparing the two expressions for $M^{-1}$, we get the (nonobvious) formula
\[
(A - BD^{-1}C)^{-1} = A^{-1} + A^{-1}B(D - CA^{-1}B)^{-1}CA^{-1}.
\]

Using this formula, we obtain another expression for the inverse of $M$ involving the Schur complements of $A$ and $D$ (see Horn and Johnson [56]):

Proposition 7.2. If $A, D$ and both Schur complements $A - BD^{-1}C$ and $D - CA^{-1}B$ are all invertible, then
\[
\begin{pmatrix} A & B \\ C & D \end{pmatrix}^{-1} = \begin{pmatrix} (A - BD^{-1}C)^{-1} & -A^{-1}B(D - CA^{-1}B)^{-1} \\ -(D - CA^{-1}B)^{-1}CA^{-1} & (D - CA^{-1}B)^{-1} \end{pmatrix}.
\]

If we set $D = I$ and change $B$ to $-B$, we get
\[
(A + BC)^{-1} = A^{-1} - A^{-1}B(I - CA^{-1}B)^{-1}CA^{-1},
\]
a formula known as the matrix inversion lemma (see Boyd and Vandenberghe [22], Appendix C.4, especially C.4.3).
7.2 Symmetric Positive Definite Matrices and Schur Complements

If we assume that our block matrix $M$ is symmetric, so that $A, D$ are symmetric and $C = B^\top$, then we see that $M$ is expressed as

$$M = \begin{pmatrix} A & B \\ B^\top & D \end{pmatrix} = \begin{pmatrix} I & BD^{-1} \\ 0 & I \end{pmatrix} \begin{pmatrix} A - BD^{-1}B^\top & 0 \\ 0 & D \end{pmatrix} \begin{pmatrix} I & BD^{-1} \\ 0 & I \end{pmatrix}^\top,$$

which shows that $M$ is similar to a block diagonal matrix (obviously, the Schur complement, $A - BD^{-1}B^\top$, is symmetric). As a consequence, we have the following version of “Schur’s trick” to check whether $M \succ 0$ for a symmetric matrix.

**Proposition 7.3.** For any symmetric matrix $M$ of the form

$$M = \begin{pmatrix} A & B \\ B^\top & C \end{pmatrix},$$

if $C$ is invertible, then the following properties hold:

1. $M \succ 0$ iff $C \succ 0$ and $A - BC^{-1}B^\top \succ 0$.
2. If $C \succ 0$, then $M \succeq 0$ iff $A - BC^{-1}B^\top \succeq 0$.

**Proof.** (1) Observe that

$$\begin{pmatrix} I & BC^{-1} \\ 0 & I \end{pmatrix}^{-1} = \begin{pmatrix} I & -BC^{-1} \\ 0 & I \end{pmatrix},$$

and we know that for any symmetric matrix $T$ and any invertible matrix $N$, the matrix $T$ is positive definite ($T \succ 0$) iff $NTN^\top$ (which is obviously symmetric) is positive definite ($NTN^\top \succ 0$). But a block diagonal matrix is positive definite iff each diagonal block is positive definite, which concludes the proof.

(2) This is because for any symmetric matrix $T$ and any invertible matrix $N$, we have $T \succeq 0$ iff $NTN^\top \succeq 0$. □

Another version of Proposition 24.3 using the Schur complement of $A$ instead of the Schur complement of $C$ also holds. The proof uses the factorization of $M$ using the Schur complement of $A$ (see Section 24.1).

**Proposition 7.4.** For any symmetric matrix $M$ of the form

$$M = \begin{pmatrix} A & B \\ B^\top & C \end{pmatrix},$$

if $A$ is invertible then the following properties hold:
(1) $M \succ 0$ iff $A \succ 0$ and $C - B^\top A^{-1}B \succ 0$.

(2) If $A \succ 0$, then $M \succeq 0$ iff $C - B^\top A^{-1}B \succeq 0$.

Here is an illustration of Proposition 24.4(2). Consider the nonlinear quadratic constraint

$$(Ax + b)^\top (Ax + b) \leq c^\top x + d,$$

were $A \in \mathbb{M}_n(\mathbb{R}), x, b, c \in \mathbb{R}^n$ and $d \in \mathbb{R}$. Since obviously $I = I_n$ is invertible and $I \succ 0$, we have

$$\begin{pmatrix} I & Ax + b \\ (Ax + b)^\top & c^\top x + d \end{pmatrix} \succeq 0$$

iff $c^\top x + d - (Ax + b)^\top (Ax + b) \succeq 0$ iff $(Ax + b)^\top (Ax + b) \leq c^\top x + d$, since the matrix (a scalar) $c^\top x + d - (Ax + b)^\top (Ax + b)$ is the Schur complement of $I$ in the above matrix.

The trick of using Schur complements to convert nonlinear inequality constraints into linear constraints on symmetric matrices involving the semidefiniteness ordering $\succeq$ is used extensively to convert nonlinear problems into semidefinite programs; see Boyd and Vandenberghe [22].

When $C$ is singular (or $A$ is singular), it is still possible to characterize when a symmetric matrix $M$ as above is positive semidefinite, but this requires using a version of the Schur complement involving the pseudo-inverse of $C$, namely $A - BC^+B^\top$ (or the Schur complement, $C - B^\top A^+B$, of $A$). We use the criterion of Proposition 23.5, which tells us when a quadratic function of the form $\frac{1}{2}x^\top Px - x^\top b$ has a minimum and what this optimum value is (where $P$ is a symmetric matrix).

### 7.3 Symmetric Positive Semidefinite Matrices and Schur Complements

We now return to our original problem, characterizing when a symmetric matrix

$$M = \begin{pmatrix} A & B \\ B^\top & C \end{pmatrix}$$

is positive semidefinite. Thus, we want to know when the function

$$f(x, y) = (x^\top, y^\top) \begin{pmatrix} A & B \\ B^\top & C \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = x^\top Ax + 2x^\top By + y^\top Cy$$

has a minimum with respect to both $x$ and $y$. If we hold $y$ constant, Proposition 23.5 implies that $f(x, y)$ has a minimum iff $A \succeq 0$ and $(I - AA^+)By = 0$, and then the minimum value is

$$f(x^*, y) = -y^\top B^\top A^+By + y^\top Cy = y^\top (C - B^\top A^+B)y.$$
Since we want $f(x, y)$ to be uniformly bounded from below for all $x, y$, we must have $(I - AA^+)B = 0$. Now, $f(x^*, y)$ has a minimum iff $C - B^TA^+B \succeq 0$. Therefore, we have established that $f(x, y)$ has a minimum over all $x, y$ iff

$$A \succeq 0, \quad (I - AA^+)B = 0, \quad C - B^TA^+B \succeq 0.$$ 

Similar reasoning applies if we first minimize with respect to $y$ and then with respect to $x$, but this time, the Schur complement $A - BC^+B^\top$ of $C$ is involved. Putting all these facts together, we get our main result:

**Theorem 7.5.** Given any symmetric matrix

$$M = \begin{pmatrix} A & B \\ B^\top & C \end{pmatrix}$$

the following conditions are equivalent:

1. $M \succeq 0$ ($M$ is positive semidefinite).

2. $A \succeq 0, \quad (I - AA^+)B = 0, \quad C - B^TA^+B \succeq 0$. 

3. $C \succeq 0, \quad (I - CC^+)B^\top = 0, \quad A - BC^+B^\top \succeq 0$.

If $M \succeq 0$ as in Theorem 24.5, then it is easy to check that we have the following factorizations (using the fact that $A^+AA^+ = A^+$ and $C^+CC^+ = C^+$):

$$\begin{pmatrix} A & B \\ B^\top & C \end{pmatrix} = \begin{pmatrix} I & BC^+ \\ 0 & I \end{pmatrix} \begin{pmatrix} A - BC^+B^\top & 0 \\ 0 & C \end{pmatrix} \begin{pmatrix} I & 0 \\ C^+B^\top & I \end{pmatrix}$$

and

$$\begin{pmatrix} A & B \\ B^\top & C \end{pmatrix} = \begin{pmatrix} I & 0 \\ B^\top A^+ & I \end{pmatrix} \begin{pmatrix} A & 0 \\ 0 & C - B^TA^+B \end{pmatrix} \begin{pmatrix} I & A^+B \\ 0 & I \end{pmatrix}.$$
Part II

Linear Optimization
Chapter 8

Convex Sets, Cones, $\mathcal{H}$-Polyhedra

8.1 What is Linear Programming?

What is *linear programming*? At first glance, one might think that this is some style of computer programming. After all, there is imperative programming, functional programming, object-oriented programming *etc.* The term linear programming is somewhat misleading, because it really refers to a method for *planning* with linear constraints, or more accurately, an *optimization method* where both the objective function and the constraints are linear.\(^{1}\)

Linear programming was created in the late 1940’s, one of the key players being George Dantzing, who invented the simplex algorithm. Kantorovitch also did some pioneering work on linear programming as early as 1939. The term *linear programming* has a military connotation because in the early 1950’s it was used as a synonym for plans or schedules for training troops, logistical supply, resource allocation, *etc.* Unfortunately the term linear programming is well established and we are stuck with it.

Interestingly, even though originally most applications of linear programming were in the field of economics and industrial engineering, linear programming has become an important tool in theoretical computer science and in the theory of algorithms. Indeed, linear programming is often an effective tool for designing approximation algorithms to solve hard problems (typically NP-hard problems). Linear programming is also the “baby version” of convex programming, a very effective methodology which has received much attention in recent years.

Our goal in these notes is to present the mathematical underpinnings of linear programming, in particular the existence of an optimal solution if a linear program is feasible and bounded, and the duality theorem in linear programming, one of the deepest results in this field. The duality theorem in linear programming also has significant algorithmic implications but we do not discuss this here. We present the simplex algorithm, the dual simplex algorithm, and the primal dual algorithm. We also describe the tableau formalism.

\(^{1}\)Again, we witness another unfortunate abuse of terminology; the constraints are in fact *affine.*
for running the simplex algorithm and its variants. A particularly nice feature of the tableau formalism is that the update of a tableau can be performed using elementary row operations identical to the operations used during the reduction of a matrix to row reduced echelon form (rref). What differs is the criterion for the choice of the pivot.

However, we do not discuss other methods such as the ellipsoid method or interior points methods. For these more algorithmic issues, we refer the reader to standard texts on linear programming. In our opinion, one of the clearest (and among the most concise!) is Matousek and Gardner [73]; Chvatal [29] and Schrijver [89] are classics. Papadimitriou and Steiglitz [80] offers a very crisp presentation in the broader context of combinatorial optimization, and Bertsimas and Tsitsiklis [17] and Vanderbei [110] are very complete.

Linear programming has to do with maximizing a linear cost function $c_1x_1 + \cdots + c_nx_n$ with respect to $m$ “linear” inequalities of the form

$$a_{i1}x_1 + \cdots + a_{in}x_n \leq b_i.$$ 

These constraints can be put together into an $m \times n$ matrix $A = (a_{ij})$, and written more concisely as

$$Ax \leq b.$$ 

For technical reasons that will appear clearer later on, it is often preferable to add the nonnegativity constraints $x_i \geq 0$ for $i = 1, \ldots, n$. We write $x \geq 0$. It is easy to show that every linear program is equivalent to another one satisfying the constraints $x \geq 0$, at the expense of adding new variables that are also constrained to be nonnegative. Let $P(A, b)$ be the set of feasible solutions of our linear program given by

$$P(A, b) = \{x \in \mathbb{R}^n \mid Ax \leq b, x \geq 0\}.$$ 

Then, there are two basic questions:

1. Is $P(A, b)$ nonempty, that is, does our linear program have a chance to have a solution?
2. Does the objective function $c_1x_1 + \cdots + c_nx_n$ have a maximum value on $P(A, b)$?

The answer to both questions can be no. But if $P(A, b)$ is nonempty and if the objective function is bounded above (on $P(A, b)$), then it can be shown that the maximum of $c_1x_1 + \cdots + c_nx_n$ is achieved by some $x \in P(A, b)$. Such a solution is called an optimal solution. Perhaps surprisingly, this result is not so easy to prove (unless one has the simplex method as its disposal). We will prove this result in full detail (see Proposition 26.1).

The reason why linear constraints are so important is that the domain of potential optimal solutions $P(A, b)$ is convex. In fact, $P(A, b)$ is a convex polyhedron which is the intersection of half-spaces cut out by affine hyperplanes. The objective function being linear is convex, and this is also a crucial fact. Thus, we are led to study convex sets, in particular those that arise from solutions of inequalities defined by affine forms, but also convex cones.
We give a brief introduction to these topics. As a reward, we provide several criteria for testing whether a system of inequalities
\[ Ax \leq b, \quad x \geq 0 \]
has a solution or not in terms of versions of the Farkas lemma (see Proposition 31.3 and Proposition 28.4). Then we give a complete proof of the strong duality theorem for linear programming (see Theorem 28.7). We also discuss the complementary slackness conditions and show that they can be exploited to design an algorithm for solving a linear program that uses both the primal problem and its dual. This algorithm known as the primal dual algorithm, although not used much nowadays, has been the source of inspiration for a whole class of approximation algorithms also known as primal dual algorithms.

We hope that these notes will be a motivation for learning more about linear programming, convex optimization, but also convex geometry. The “bible” in convex optimization is Boyd and Vandenberghe [22], and one of the best sources for convex geometry is Ziegler [114]. This is a rather advanced text, so the reader may want to begin with Gallier [45].

8.2 Affine Subsets, Convex Sets, Affine Hyperplanes, Half-Spaces

We view \( \mathbb{R}^n \) as consisting of column vectors \((n \times 1)\) matrices. As usual, row vectors represent linear forms, that is linear maps \( \varphi : \mathbb{R}^n \to \mathbb{R} \), in the sense that the row vector \( y \) (a \( 1 \times n \) matrix) represents the linear form \( \varphi \) if \( \varphi(x) = yx \) for all \( x \in \mathbb{R}^n \). We denote the space of linear forms (row vectors) by \((\mathbb{R}^n)^*\).

Recall that a linear combination of vectors in \( \mathbb{R}^n \) is an expression
\[ \lambda_1 x_1 + \cdots + \lambda_m x_m \]
where \( x_1, \ldots, x_m \in \mathbb{R}^n \) and where \( \lambda_1, \ldots, \lambda_m \) are arbitrary scalars in \( \mathbb{R} \). Given a sequence of vectors \( S = (x_1, \ldots, x_m) \) with \( x_i \in \mathbb{R}^n \), the set of all linear combinations of the vectors in \( S \) is the smallest (linear) subspace containing \( S \) called the linear span of \( S \), and denoted \( \text{span}(S) \). A linear subspace of \( \mathbb{R}^n \) is any nonempty subset of \( \mathbb{R}^n \) closed under linear combinations.

An affine combination of vectors in \( \mathbb{R}^n \) is an expression
\[ \lambda_1 x_1 + \cdots + \lambda_m x_m \]
where \( x_1, \ldots, x_m \in \mathbb{R}^n \) and where \( \lambda_1, \ldots, \lambda_m \) are scalars in \( \mathbb{R} \) satisfying the condition
\[ \lambda_1 + \cdots + \lambda_m = 1. \]

Given a sequence of vectors \( S = (x_1, \ldots, x_m) \) with \( x_i \in \mathbb{R}^n \), the set of all affine combinations of the vectors in \( S \) is the smallest affine subspace containing \( S \) called the affine hull of \( S \) and denoted \( \text{aff}(S) \).
CHAPTER 8. CONVEX SETS, CONES, $\mathcal{H}$-POLYHEDRA

(a) (b)

Figure 8.1: (a) A convex set; (b) A nonconvex set

Definition 8.1. An affine subspace $A$ of $\mathbb{R}^n$ is any subset of $\mathbb{R}^n$ closed under affine combinations.

If $A$ is a nonempty affine subset of $\mathbb{R}^n$, then it can be shown that $V_A = \{a - b \mid a, b \in A\}$ is a linear subspace of $\mathbb{R}^n$ called the direction of $A$, and that

$$A = a + V_A = \{a + v \mid v \in V_A\}$$

for any $a \in A$. The dimension of a nonempty affine subspace $A$ is the dimension of its direction $V_A$.

Convex combinations are affine combinations $\lambda_1 x_1 + \cdots + \lambda_m x_m$ satisfying the extra condition that $\lambda_i \geq 0$ for $i = 1, \ldots, m$. A convex set is defined as follows.

Definition 8.2. A subset $V$ of $\mathbb{R}^n$ is convex if for any two points $a, b \in V$, we have $c \in V$ for every point $c = (1 - \lambda)a + \lambda b$, with $0 \leq \lambda \leq 1$ ($\lambda \in \mathbb{R}$). Given any two points $a, b$, the notation $[a, b]$ is often used to denote the line segment between $a$ and $b$, that is,

$$[a, b] = \{c \in \mathbb{R}^n \mid c = (1 - \lambda)a + \lambda b, \ 0 \leq \lambda \leq 1\},$$

and thus a set $V$ is convex if $[a, b] \subseteq V$ for any two points $a, b \in V$ ($a = b$ is allowed). The dimension of a convex set $V$ is the dimension of its affine hull $\text{aff}(A)$.

The empty set is trivially convex, every one-point set $\{a\}$ is convex, and the entire affine space $\mathbb{R}^n$ is convex.

It is obvious that the intersection of any family (finite or infinite) of convex sets is convex.

Definition 8.3. Given any (nonempty) subset $S$ of $\mathbb{R}^n$, the smallest convex set containing $S$ is denoted by $\text{conv}(S)$ and called the convex hull of $S$ (it is the intersection of all convex sets containing $S$).
A good understanding of what \( \text{conv}(S) \) is, and good methods for computing it, are essential. We have the following simple but crucial result.

**Proposition 8.1.** For any family \( S = (a_i)_{i \in I} \) of points in \( \mathbb{R}^n \), the set \( V \) of convex combinations \( \sum_{i \in I} \lambda_i a_i \) (where \( \sum_{i \in I} \lambda_i = 1 \) and \( \lambda_i \geq 0 \)) is the convex hull \( \text{conv}(S) \) of \( S = (a_i)_{i \in I} \).

It is natural to wonder whether Proposition 25.1 can be sharpened in two directions:

1. Is it possible to have a fixed bound on the number of points involved in the convex combinations?
2. Is it necessary to consider convex combinations of all points, or is it possible to consider only a subset with special properties?

The answer is yes in both cases. In Case 1, Carathéodory’s theorem asserts that it is enough to consider convex combinations of \( n + 1 \) points. For example, in the plane \( \mathbb{R}^2 \), the convex hull of a set \( S \) of points is the union of all triangles (interior points included) with vertices in \( S \). In Case 2, the theorem of Krein and Milman asserts that a convex set that is also compact is the convex hull of its extremal points (given a convex set \( S \), a point \( a \in S \) is extremal if \( S - \{a\} \) is also convex).

We will not prove these theorems here, but we invite the reader to consult Gallier [45] or Berger [10].

Convex sets also arise as half-spaces cut out by affine hyperplanes.

**Definition 8.4.** An affine form \( \varphi : \mathbb{R}^n \to \mathbb{R} \) is defined by some linear form \( c \in (\mathbb{R}^n)^* \) and some scalar \( \beta \in \mathbb{R} \) so that

\[
\varphi(x) = cx + \beta \quad \text{for all } x \in \mathbb{R}^n.
\]

If \( c \neq 0 \), the affine form \( \varphi \) specified by \((c, \beta)\) defines the affine hyperplane (for short hyperplane) \( H(\varphi) \) given by

\[
H(\varphi) = \{ x \in \mathbb{R}^n \mid \varphi(x) = 0 \} = \{ x \in \mathbb{R}^n \mid cx + \beta = 0 \},
\]

and the two (closed) half-spaces

\[
H_+(\varphi) = \{ x \in \mathbb{R}^n \mid \varphi(x) \geq 0 \} = \{ x \in \mathbb{R}^n \mid cx + \beta \geq 0 \},
\]

\[
H_-(\varphi) = \{ x \in \mathbb{R}^n \mid \varphi(x) \leq 0 \} = \{ x \in \mathbb{R}^n \mid cx + \beta \leq 0 \}.
\]

When \( \beta = 0 \), we call \( H \) a linear hyperplane.

Both \( H_+(\varphi) \) and \( H_-(\varphi) \) are convex and \( H = H_+(\varphi) \cap H_-(\varphi) \).

For example, \( \varphi : \mathbb{R}^2 \to \mathbb{R} \) with \( \varphi(x,y) = 2x + y + 3 \) is an affine form defining the line given by the equation \( y = -2x - 3 \). Another example of an affine form is \( \varphi : \mathbb{R}^3 \to \mathbb{R} \) with \( \varphi(x,y,z) = x + y + z - 1 \); this affine form defines the plane given by the equation \( x + y + z = 1 \), which is the plane through the points \((0,0,1),(0,1,0)\), and \((1,0,0)\). Both of these hyperplanes are illustrated in Figure 25.2.
Figure 8.2: Figure i. illustrates the hyperplane $H(\varphi)$ for $\varphi(x,y) = 2x + y + 3$, while Figure ii. illustrates the hyperplane $H(\varphi)$ for $\varphi(x,y,z) = x + y + z - 1$.

For any two vector $x, y \in \mathbb{R}^n$ with $x = (x_1, \ldots, x_n)$ and $y = (y_1, \ldots, y_n)$ we write $x \leq y$ iff $x_i \leq y_i$ for $i = 1, \ldots, n$, and $x \geq y$ iff $y \leq x$. In particular $x \geq 0$ iff $x_i \geq 0$ for $i = 1, \ldots, n$.

Certain special types of convex sets called cones and $H$-polyhedra play an important role. The set of feasible solutions of a linear program is an $H$-polyhedron, and cones play a crucial role in the proof of Proposition 26.1 and in the Farkas–Minkowski proposition (Proposition 28.2).

### 8.3 Cones, Polyhedral Cones, and $H$-Polyhedra

Cones and polyhedral cones are defined as follows.

**Definition 8.5.** Given a nonempty subset $S \subseteq \mathbb{R}^n$, the cone $C = \text{cone}(S)$ spanned by $S$ is the convex set

$$\text{cone}(S) = \left\{ \sum_{i=1}^{k} \lambda_i u_i, \ u_i \in S, \lambda_i \in \mathbb{R}, \ \lambda_i \geq 0 \right\},$$

of positive combinations of vectors from $S$. If $S$ consists of a finite set of vector, the cone $C = \text{cone}(S)$ is called a polyhedral cone. Figure 25.3 illustrates a polyhedral cone.

Note that if some nonzero vector $u$ belongs to a cone $C$, then $\lambda u \in C$ for all $\lambda \geq 0$, that is, the ray $\{ \lambda u \mid \lambda \geq 0 \}$ belongs to $C$.

**Remark:** The cones (and polyhedral cones) of Definition 25.5 are always convex. For this reason we use the simpler terminology cone instead of convex cone. However, there are more
8.3. CONES, POLYHEDRAL CONES, AND $\mathcal{H}$-POLYHEDRA

Figure 8.3: Let $S = \{(0,0,1), (1,0,1), (1,1,1), (0,1,1)\}$. The polyhedral cone, cone($S$), is the solid “pyramid” with apex at the origin and square cross sections.

general kinds of cones that are not convex (for example, a union of polyhedral cones or the linear cone generated by the curve in Figure 25.4), and if we were dealing with those we would refer to the cones of Definition 25.5 as convex cones.

**Definition 8.6.** An $\mathcal{H}$-polyhedron, for short a polyhedron, is any subset $P = \bigcap_{i=1}^{s} C_i$ of $\mathbb{R}^n$ defined as the intersection of a finite number $s$ of closed half-spaces $C_i$. An example of an $\mathcal{H}$-polyhedron is shown in Figure 25.6. An $\mathcal{H}$-polytope is a bounded $\mathcal{H}$-polyhedron, which means that there is a closed ball $B_r(x)$ of center $x$ and radius $r > 0$ such that $P \subseteq B_r(x)$. An example of a $\mathcal{H}$-polytope is shown in Figure 25.5.

By convention, we agree that $\mathbb{R}^n$ itself is an $\mathcal{H}$-polyhedron.

**Remark:** The $\mathcal{H}$-polyhedra of Definition 25.6 are always convex. For this reason, as in the case of cones we use the simpler terminology $\mathcal{H}$-polyhedron instead of convex $\mathcal{H}$-polyhedron. In algebraic topology, there are more general polyhedra that are not convex.

It can be shown that an $\mathcal{H}$-polytope $P$ is equal to the convex hull of finitely many points (the extreme points of $P$). This is a nontrivial result whose proof takes a significant amount of work; see Gallier [45] and Ziegler [114].

An unbounded $\mathcal{H}$-polyhedron is not equal to the convex hull of finite set of points. To obtain an equivalent notion we introduce the notion of a $\mathcal{V}$-polyhedron.
Figure 8.4: Let $S$ be a planar curve in $z = 1$. The linear cone of $S$, consisting of all half rays connecting $S$ to the origin, is not convex.

**Definition 8.7.** A $\mathcal{V}$-polyhedron is any convex subset $A \subseteq \mathbb{R}^n$ of the form

$$A = \text{conv}(Y) + \text{cone}(V) = \{a + v \mid a \in \text{conv}(Y), \ v \in \text{cone}(V)\},$$

where $Y \subseteq \mathbb{R}^n$ and $V \subseteq \mathbb{R}^n$ are finite (possibly empty).

When $V = \emptyset$ we simply have a polytope, and when $Y = \emptyset$ or $Y = \{0\}$, we simply have a cone.

It can be shown that every $\mathcal{H}$-polyhedron is a $\mathcal{V}$-polyhedron and conversely. This is one of the major theorems in the theory of polyhedra, and its proof is nontrivial. For a complete proof, see Gallier [45] and Ziegler [114].

Every polyhedral cone is closed. This is an important fact that is used in the proof of several other key results such as Proposition 26.1 and the Farkas–Minkowski proposition (Proposition 28.2).

Although it seems obvious that a polyhedral cone should be closed, a rigorous proof is not entirely trivial.

Indeed, the fact that a polyhedral cone is closed relies crucially on the fact that $C$ is spanned by a finite number of vectors, because the cone generated by an infinite set may not be closed. For example, consider the closed disk $D \subseteq \mathbb{R}^2$ of center $(0, 1)$ and radius 1, which is tangent to the $x$-axis at the origin. Then the cone($D$) consists of the open upper half-plane plus the origin $(0, 0)$, but this set is not closed.
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![Figure 8.5: An icosahedron is an example of an H-polytope.](image)

**Proposition 8.2.** Every polyhedral cone \( C \) is closed.

**Proof.** This is proved by showing that

1. Every primitive cone is closed.

2. A polyhedral cone \( C \) is the union of finitely many primitive cones, where a primitive cone is a polyhedral cone spanned by linearly independent vectors.

Assume that \((a_1, \ldots, a_m)\) are linearly independent vectors in \( \mathbb{R}^n \), and consider any sequence \((x^{(k)})_{k \geq 0}\)

\[
x^{(k)} = \sum_{i=1}^{m} \lambda_i^{(k)} a_i
\]

of vectors in the primitive cone \( \text{cone}\{(a_1, \ldots, a_m)\} \), which means that \( \lambda_i^{(k)} \geq 0 \) for \( i = 1, \ldots, m \) and all \( k \geq 0 \). The vectors \( x^{(k)} \) belong to the subspace \( U \) spanned by \( (a_1, \ldots, a_m) \), and \( U \) is closed. Assume that the sequence \( (x^{(k)})_{k \geq 0} \) converges to a limit \( x \in \mathbb{R}^n \). Since \( U \) is closed and \( x^{(k)} \in U \) for all \( k \geq 0 \), we have \( x \in U \). If we write \( x = x_1a_1 + \cdots + x_ma_m \), we would like to prove that \( x_i \geq 0 \) for \( i = 1, \ldots, m \). The sequence the \((x^{(k)})_{k \geq 0}\) converges to \( x \) iff

\[
\lim_{k \to \infty} \|x^{(k)} - x\| = 0,
\]

iff

\[
\lim_{k \to \infty} \left( \sum_{i=1}^{m} |\lambda_i^{(k)} - x_i|^2 \right)^{1/2} = 0
\]

iff

\[
\lim_{k \to \infty} \lambda_i^{(k)} = x_i, \quad i = 1, \ldots, m.
\]

Since \( \lambda_i^{(k)} \geq 0 \) for \( i = 1, \ldots, m \) and all \( k \geq 0 \), we have \( x_i \geq 0 \) for \( i = 1, \ldots, m \), so \( x \in \text{cone}(\{a_1, \ldots, a_m\}) \).
Figure 8.6: The “triangular trough” determined by the inequalities \( y - z \leq 0, \ y + z \geq 0, \) and \(-2 \leq x \leq 2\) is an \( H\)-polyhedron and an \( V\)-polyhedron, where \( Y = \{(2,0,0), (-2,0,0)\} \) and \( V = \{(0,1,1), (0,-1,1)\} \).

Next, assume that \( x \) belongs to the polyhedral cone \( C \). Consider a positive combination

\[ x = \lambda_1 a_1 + \cdots + \lambda_k a_k, \]  

(\( \ast_1 \))

for some nonzero \( a_1, \ldots, a_k \in C \), with \( \lambda_i \geq 0 \) and with \( k \) minimal. Since \( k \) is minimal, we must have \( \lambda_i > 0 \) for \( i = 1, \ldots, k \). We claim that \( (a_1, \ldots, a_k) \) are linearly independent.

If not, there is some nontrivial linear combination

\[ \mu_1 a_1 + \cdots + \mu_k a_k = 0, \]  

(\( \ast_2 \))

and since the \( a_i \) are nonzero, \( \mu_j \neq 0 \) for some at least some \( j \). We may assume that \( \mu_j < 0 \) for some \( j \) (otherwise, we consider the family \(-\mu_i)_{1 \leq i \leq k}\), so let

\[ J = \{ j \in \{1, \ldots, k\} \mid \mu_j < 0 \}. \]

For any \( t \in \mathbb{R} \), since \( x = \lambda_1 a_1 + \cdots + \lambda_k a_k \), using \( \ast_2 \) we get

\[ x = (\lambda_1 + t \mu_1) a_1 + \cdots + (\lambda_k + t \mu_k) a_k, \]  

(\( \ast_3 \))
and if we pick

\[ t = \min_{j \in J} \left( -\frac{\lambda_j}{\mu_j} \right) \geq 0, \]

we have \((\lambda_i + t\mu_i) \geq 0\) for \(i = 1, \ldots, k\); but \(\lambda_j + t\mu_j = 0\) for some \(j \in J\), so \((*3)\) is an expression of \(x\) with less that \(k\) nonzero coefficients, contradicting the minimality of \(k\) in \((*1)\). Therefore, \((a_1, \ldots, a_k)\) are linearly independent.

Since a polyhedral cone \(C\) is spanned by finitely many vectors, there are finitely many primitive cones (corresponding to linearly independent subfamilies), and since every \(x \in C\), belongs to some primitive cone, \(C\) is the union of a finite number of primitive cones. Since every primitive cone is closed, as a union of finitely many closed sets, \(C\) itself is closed.

The above facts are also proved in Matousek and Gardner [73] (Chapter 6, Section 5, Lemma 6.5.3, 6.5.4, and 6.5.5).

Another way to prove that a polyhedral cone \(C\) is closed is to show that \(C\) is also a \(\mathcal{H}\)-polyhedron. This takes even more work; see Gallier [45] (Chapter 4, Section 4, Proposition 4.16). Yet another proof is given in Lax [67] (Chapter 13, Theorem 1).
Chapter 9

Linear Programs

9.1 Linear Programs, Feasible Solutions, Optimal Solutions

The purpose of linear programming is to solve the following type of optimization problem.

Definition 9.1. A linear program $(P)$ is the following kind of optimization problem:

\[
\text{maximize } \quad cx \\
\text{subject to } \\
a_1x \leq b_1 \\
\vdots \\
a_mx \leq b_m \\
x \geq 0,
\]

where $x \in \mathbb{R}^n$, $c, a_1, \ldots, a_m \in (\mathbb{R}^n)^*$, $b_1, \ldots, b_m \in \mathbb{R}$.

The linear form $c$ defines the objective function $x \mapsto cx$ of the program $(P)$ (from $\mathbb{R}^n$ to $\mathbb{R}$), and the inequalities $a_ix \leq b_i$ and $x_j \geq 0$ are called the constraints of the linear program $(P)$.

If we define the $m \times n$ matrix

\[
A = \begin{pmatrix} a_1 \\ \vdots \\ a_m \end{pmatrix}
\]

whose rows are the row vectors $a_1, \ldots, a_m$ and $b$ as the column vector

\[
b = \begin{pmatrix} b_1 \\ \vdots \\ b_m \end{pmatrix},
\]
the \( m \) inequality constraints \( a_i x \leq b_i \) can be written in matrix form as

\[
Ax \leq b.
\]

Thus the linear program \((P)\) can also be stated as the linear program \((P)\):

\[
\begin{align*}
\text{maximize} \quad & cx \\
\text{subject to} \quad & Ax \leq b \quad \text{and} \quad x \geq 0.
\end{align*}
\]

Here is an explicit example of a linear program of type \((P)\):

**Example 9.1.**

\[
\begin{align*}
\text{maximize} \quad & x_1 + x_2 \\
\text{subject to} \quad & x_2 - x_1 \leq 1 \\
& x_1 + 6x_2 \leq 15 \\
& 4x_1 - x_2 \leq 10 \\
& x_1 \geq 0, \ x_2 \geq 0,
\end{align*}
\]

and in matrix form

\[
\begin{align*}
\text{maximize} \quad & (1 \ 1) \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \\
\text{subject to} \quad & \begin{pmatrix} -1 & 1 \\ 1 & 6 \\ 4 & -1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \leq \begin{pmatrix} 1 \\ 15 \\ 10 \end{pmatrix} \\
& x_1 \geq 0, \ x_2 \geq 0.
\end{align*}
\]

It turns out that \( x_1 = 3, x_2 = 2 \) yields the maximum of the objective function \( x_1 + x_2 \), which is 5. This is illustrated in Figure 26.1. Observe that the set of points that satisfy the above constraints is a convex region cut out by half planes determined by the lines of equations

\[
\begin{align*}
x_2 - x_1 &= 1 \\
x_1 + 6x_2 &= 15 \\
4x_1 - x_2 &= 10 \\
x_1 &= 0 \\
x_2 &= 0.
\end{align*}
\]
In general, each constraint $a_i x \leq b_i$ corresponds to the affine form $\varphi_i$ given by $\varphi_i(x) = a_i x - b_i$ and defines the half-space $H_-(\varphi_i)$, and each inequality $x_j \geq 0$ defines the half-space $H_+(x_j)$. The intersection of these half-spaces is the set of solutions of all these constraints. It is a (possibly empty) $\mathcal{H}$-polyhedron denoted $\mathcal{P}(A,b)$.

**Definition 9.2.** If $\mathcal{P}(A,b) = \emptyset$, we say that the linear program $(P)$ has no feasible solution, and otherwise any $x \in \mathcal{P}(A,b)$ is called a feasible solution of $(P)$.

The linear program shown in Example 26.2 obtained by reversing the direction of the inequalities $x_2 - x_1 \leq 1$ and $4x_1 - x_2 \leq 10$ in the linear program of Example 26.1 has no feasible solution; see Figure 26.2.

**Example 9.2.**

\[
\text{maximize} \quad x_1 + x_2 \\
\text{subject to} \quad \begin{align*}
x_1 - x_2 & \leq -1 \\
x_1 + 6x_2 & \leq 15 \\
x_2 - 4x_1 & \leq -10 \\
x_1 & \geq 0, \ x_2 \geq 0.
\end{align*}
\]

Assume $\mathcal{P}(A,b) \neq \emptyset$, so that the linear program $(P)$ has a feasible solution. In this case, consider the image $\{cx \in \mathbb{R} \mid x \in \mathcal{P}(A,b)\}$ of $\mathcal{P}(A,b)$ under the objective function $x \mapsto cx$. 
Definition 9.3. If the set \( \{cx \in \mathbb{R} \mid x \in \mathcal{P}(A, b)\} \) is unbounded above, then we say that the linear program \((P)\) is \emph{unbounded}.

The linear program shown in Example 26.3 obtained from the linear program of Example 26.1 by deleting the constraints \( 4x_1 - x_2 \leq 10 \) and \( x_1 + 6x_2 \leq 15 \) is unbounded.

Example 9.3.

\[
\begin{align*}
\text{maximize} & \quad x_1 + x_2 \\
\text{subject to} & \quad x_2 - x_1 \leq 1 \\
& \quad x_1 \geq 0, \ x_2 \geq 0.
\end{align*}
\]

Otherwise, we will prove shortly that if \( \mu \) is the least upper bound of the set \( \{cx \in \mathbb{R} \mid x \in \mathcal{P}(A, b)\} \), then there is some \( p \in \mathcal{P}(A, b) \) such that

\[ cp = \mu, \]

that is, the objective function \( x \mapsto cx \) has a maximum value \( \mu \) on \( \mathcal{P}(A, b) \) which is achieved by some \( p \in \mathcal{P}(A, b) \).

Definition 9.4. If the set \( \{cx \in \mathbb{R} \mid x \in \mathcal{P}(A, b)\} \) is nonempty and bounded above, any point \( p \in \mathcal{P}(A, b) \) such that \( cp = \max \{cx \in \mathbb{R} \mid x \in \mathcal{P}(A, b)\} \) is called an \emph{optimal solution} (or \emph{optimum}) of \((P)\). Optimal solutions are often denoted by an upper \( * \); for example, \( p^* \).
The linear program of Example 26.1 has a unique optimal solution \((3, 2)\), but observe that the linear program of Example 26.4 in which the objective function is \((1/6)x_1 + x_2\) has infinitely many optimal solutions; the maximum of the objective function is \(15/6\) which occurs along the points of orange boundary line in Figure 26.1.

**Example 9.4.**

\[
\begin{align*}
\text{maximize} & \quad \frac{1}{6}x_1 + x_2 \\
\text{subject to} & \quad x_2 - x_1 \leq 1 \\
& \quad x_1 + 6x_2 \leq 15 \\
& \quad 4x_1 - x_2 \leq 10 \\
& \quad x_1 \geq 0, x_2 \geq 0.
\end{align*}
\]

The proof that if the set \(\{cx \in \mathbb{R} \mid x \in \mathcal{P}(A, b)\}\) is nonempty and bounded above, then there is an optimal solution \(p \in \mathcal{P}(A, b)\), is not as trivial as it might seem. It relies on the fact that a polyhedral cone is closed, a fact that was shown in Section 25.3.

We also use a trick that makes the proof simpler, which is that a linear program \((P)\) with inequality constraints \(Ax \leq b\)

\[
\begin{align*}
\text{maximize} & \quad cx \\
\text{subject to} & \quad Ax \leq b \text{ and } x \geq 0,
\end{align*}
\]

is equivalent to the linear program \((P_2)\) with equality constraints

\[
\begin{align*}
\text{maximize} & \quad \hat{c} \hat{x} \\
\text{subject to} & \quad \hat{A}\hat{x} = b \text{ and } \hat{x} \geq 0,
\end{align*}
\]

where \(\hat{A}\) is an \(m \times (n + m)\) matrix, \(\hat{c}\) is a linear form in \((\mathbb{R}^{n+m})^*\), and \(\hat{x} \in \mathbb{R}^{n+m}\), given by

\[
\hat{A} = \begin{pmatrix} A & I_m \end{pmatrix}, \quad \hat{c} = \begin{pmatrix} c & 0_m^\top \end{pmatrix}, \quad \text{and} \quad \hat{x} = \begin{pmatrix} x \\ z \end{pmatrix},
\]

with \(x \in \mathbb{R}^n\) and \(z \in \mathbb{R}^m\).

Indeed, \(\hat{A}\hat{x} = b\) and \(\hat{x} \geq 0\) iff

\[
Ax + z = b, \quad x \geq 0, z \geq 0,
\]

iff

\[
Ax \leq b, \quad x \geq 0,
\]

and \(\hat{c}\hat{x} = cx\).
The variables \( z \) are called **slack variables**, and a linear program of the form \((P_2)\) is called a linear program in **standard form**.

The result of converting the linear program of Example 26.4 to standard form is the program shown in Example 26.5.

**Example 9.5.**

\[
\begin{align*}
\text{maximize} \quad & \frac{1}{6} x_1 + x_2 \\
\text{subject to} \quad & x_2 - x_1 + z_1 = 1 \\
& x_1 + 6x_2 + z_2 = 15 \\
& 4x_1 - x_2 + z_3 = 10 \\
& x_1 \geq 0, \; x_2 \geq 0, \; z_1 \geq 0, \; z_2 \geq 0, \; z_3 \geq 0.
\end{align*}
\]

We can now prove that if a linear program has a feasible solution and is bounded, then it has an optimal solution.

**Proposition 9.1.** Let \((P_2)\) be a linear program in standard form, with equality constraint \(Ax = b\). If \(\mathcal{P}(A, b)\) is nonempty and bounded above, and if \(\mu\) is the least upper bound of the set \(\{cx \in \mathbb{R} \mid x \in \mathcal{P}(A, b)\}\), then there is some \(p \in \mathcal{P}(A, b)\) such that \(cp = \mu\), that is, the objective function \(x \mapsto cx\) has a maximum value \(\mu\) on \(\mathcal{P}(A, b)\) which is achieved by some optimum solution \(p \in \mathcal{P}(A, b)\).

**Proof.** Since \(\mu = \sup \{cx \in \mathbb{R} \mid x \in \mathcal{P}(A, b)\}\), there is a sequence \((x^{(k)})_{k \geq 0}\) of vectors \(x^{(k)} \in \mathcal{P}(A, b)\) such that \(\lim_{k \to \infty} cx^{(k)} = \mu\). In particular, if we write \(x^{(k)} = (x_1^{(k)}, \ldots, x_n^{(k)})\) we have \(x_j^{(k)} \geq 0\) for \(j = 1, \ldots, n\) and for all \(k \geq 0\). Let \(\tilde{A}\) be the \((m+1) \times n\) matrix

\[
\tilde{A} = \begin{pmatrix} c \ A \end{pmatrix},
\]

and consider the sequence \((\tilde{A}x^{(k)})_{k \geq 0}\) of vectors \(\tilde{A}x^{(k)} \in \mathbb{R}^{m+1}\). We have

\[
\tilde{A}x^{(k)} = \begin{pmatrix} c \\ A \end{pmatrix} x^{(k)} = \begin{pmatrix} cx^{(k)} \\ Ax^{(k)} \end{pmatrix} = \begin{pmatrix} c \ x^{(k)} \\ b \end{pmatrix},
\]

since by hypothesis \(x^{(k)} \in \mathcal{P}(A, b)\), and the constraints are \(Ax = b\) and \(x \geq 0\). Since by hypothesis \(\lim_{k \to \infty} cx^{(k)} = \mu\), the sequence \((\tilde{A}x^{(k)})_{k \geq 0}\) converges to the vector \(\begin{pmatrix} \mu \\ b \end{pmatrix}\). Now, observe that each vector \(\tilde{A}x^{(k)}\) can be written as the convex combination

\[
\tilde{A}x^{(k)} = \sum_{j=1}^{n} x_j^{(k)} \tilde{A}^j,
\]
with \( a_j^{(k)} \geq 0 \) and where \( \tilde{A}^j \in \mathbb{R}^{m+1} \) is the \( j \)th column of \( \tilde{A} \). Therefore, \( \tilde{A}x^{(k)} \) belongs to the polyhedral cone
\[
C = \text{cone}(\tilde{A}^1, \ldots, \tilde{A}^n) = \{ \tilde{A}x \mid x \in \mathbb{R}^n, x \geq 0 \},
\]
and since by Proposition 25.2 this cone is closed, \( \lim_{k \to \infty} \tilde{A}x^{(k)} \in C \), which means that there is some \( u \in \mathbb{R}^n \) with \( u \geq 0 \) such that
\[
\begin{pmatrix} u \\ b \end{pmatrix} = \lim_{k \to \infty} \tilde{A}x^{(k)} = \tilde{A}u = \begin{pmatrix} cu \\ Au \end{pmatrix},
\]
that is, \( cu = \mu \) and \( Au = b \). Hence, \( u \) is an optimal solution of \((P_2)\). \(\square\)

The next question is, how do we find such an optimal solution? It turns out that for linear programs in standard form where the constraints are of the form \( Ax = b \) and \( x \geq 0 \), there are always optimal solutions of a special type called basic feasible solutions.

## 9.2 Basic Feasible Solutions and Vertices

If the system \( Ax = b \) has a solution and if some row of \( A \) is a linear combination of other rows, then the corresponding equation is redundant, so we may assume that the rows of \( A \) are linearly independent; that is, we may assume that \( A \) has rank \( m \), so \( m \leq n \).

If \( A \) is an \( m \times n \) matrix, for any nonempty subset \( K \) of \( \{1, \ldots, n\} \), let \( A_K \) be the submatrix of \( A \) consisting of the columns of \( A \) whose indices belong to \( K \). We denote the \( j \)th column of the matrix \( A \) by \( A^j \).

**Definition 9.5.** Given a linear program \((P_2)\)

\[
\begin{align*}
\text{maximize} & \quad cx \\
\text{subject to} & \quad Ax = b \text{ and } x \geq 0,
\end{align*}
\]

where \( A \) has rank \( m \), a vector \( x \in \mathbb{R}^n \) is a basic feasible solution of \((P)\) if \( x \in \mathcal{P}(A, b) \neq \emptyset \), and if there is some subset \( K \) of \( \{1, \ldots, n\} \) of size \( m \) such that

(1) The matrix \( A_K \) is invertible (that is, the columns of \( A_K \) are linearly independent).

(2) \( x_j = 0 \) for all \( j \notin K \).

The subset \( K \) is called a basis of \( x \). Every index \( k \in K \) is called basic, and every index \( j \notin K \) is called nonbasic. Similarly, the columns \( A^k \) corresponding to indices \( k \in K \) are called basic, and the columns \( A^j \) corresponding to indices \( j \notin K \) are called nonbasic. The variables corresponding to basic indices \( k \in K \) are called basic variables, and the variables corresponding to indices \( j \notin K \) are called nonbasic.
For example, the linear program
\[
\begin{align*}
\text{maximize} & \quad x_1 + x_2 \\
\text{subject to} & \quad x_1 + x_2 + x_3 = 1 \quad \text{and} \quad x_1 \geq 0, \ x_2 \geq 0, \ x_3 \geq 0,
\end{align*}
\]
has three basic feasible solutions; the basic feasible solution \( K = \{1\} \) corresponds to the point \((1,0,0)\); the basic feasible solution \( K = \{2\} \) corresponds to the point \((0,1,0)\); the basic feasible solution \( K = \{3\} \) corresponds to the point \((0,0,1)\). Each of these points corresponds to the vertices of the slanted purple triangle illustrated in Figure 26.3. The vertices \((1,0,0)\) and \((0,1,0)\) optimize the objective function with a value of 1.

We now show that if the standard linear program \((P_2)\) as in Definition 26.5 has some feasible solution and is bounded above, then some basic feasible solution is an optimal solution. We follow Matousek and Gardner [73] (Chapter 4, Section 2, Theorem 4.2.3).

First we obtain a more convenient characterization of a basic feasible solution.

**Proposition 9.2.** Given any standard linear program \((P_2)\) where \( Ax = b \) and \( A \) is an \( m \times n \) matrix of rank \( m \), for any feasible solution \( x \), if \( J_\succ = \{ j \in \{1, \ldots, n\} \mid x_j > 0 \} \), then \( x \) is a basic feasible solution iff the columns of the matrix \( A_{J_\succ} \) are linearly independent.

**Proof.** If \( x \) is a basic feasible solution then there is some subset \( K \subseteq \{1, \ldots, n\} \) of size \( m \) such that the columns of \( A_K \) are linearly independent and \( x_j = 0 \) for all \( j \notin K \), so by definition \( J_\succ \subseteq K \), which implies that the columns of the matrix \( A_{J_\succ} \) are linearly independent.

Conversely, assume that \( x \) is a feasible solution such that the columns of the matrix \( A_{J_\succ} \) are linearly independent. If \( |J_\succ| = m \), we are done since we can pick \( K = J_\succ \) and then \( x \)
is a basic feasible solution. If $|J_\succ| < m$, we can extend $J_\succ$ to an $m$-element subset $K$ by adding $m - |J_\succ|$ column indices so that the columns of $A_K$ are linearly independent, which is possible since $A$ has rank $m$. 

Next we prove that if a linear program in standard form has any feasible solution $x_0$ and is bounded above, then it has some basic feasible solution $\tilde{x}$ which is as good as $x_0$, in the sense that $c\tilde{x} \geq cx_0$.

**Proposition 9.3.** Let $(P_2)$ be any standard linear program with objective function $cx$, where $Ax = b$ and $A$ is an $m \times n$ matrix of rank $m$. If $(P_2)$ is bounded above and if $x_0$ is some feasible solution of $(P_2)$, then there is some basic feasible solution $\tilde{x}$ such that $c\tilde{x} \geq cx_0$.

**Proof.** Among the feasible solutions $x$ such that $cx \geq cx_0$ ($x_0$ is one of them) pick one with the maximum number of coordinates $x_j$ equal to 0, say $\tilde{x}$. Let $K = J_\succ = \{j \in \{1, \ldots, n\} : \tilde{x}_j > 0\}$ and let $s = |K|$. We claim that $\tilde{x}$ is a basic feasible solution, and by construction $c\tilde{x} \geq cx_0$.

If the columns of $A_K$ are linearly independent, then by Proposition 26.2 we know that $\tilde{x}$ is a basic feasible solution and we are done.

Otherwise, the columns of $A_K$ are linearly dependent, so there is some nonzero vector $v = (v_1, \ldots, v_s)$ such that $A_K v = 0$. Let $w \in \mathbb{R}^n$ be the vector obtained by extending $v$ by setting $w_j = 0$ for all $j \notin K$. By construction,

$$Aw = A_K v = 0.$$ 

We will derive a contradiction by exhibiting a feasible solution $x(t_0)$ such that $cx(t_0) \geq cx_0$ with more zero coordinates than $\tilde{x}$.

For this we claim that we may assume that $w$ satisfies the following two conditions:

1. $cw \geq 0$.
2. There is some $j \in K$ such that $w_j < 0$.

If $cw = 0$ and if Condition (2) fails, since $w \neq 0$, we have $w_j > 0$ for some $j \in K$, in which case we can use $-w$, for which $w_j < 0$.

If $cw < 0$ then $c(-w) > 0$, so we may assume that $cw > 0$. If $w_j > 0$ for all $j \in K$, since $\tilde{x}$ is feasible $\tilde{x} \geq 0$, and so $x(t) = \tilde{x} + tw \geq 0$ for all $t \geq 0$. Furthermore, since $Aw = 0$ and $\tilde{x}$ is feasible, we have

$$Ax(t) = A\tilde{x} + tAw = b,$$

and thus $x(t)$ is feasible for all $t \geq 0$. We also have

$$cx(t) = c\tilde{x} + tcw.$$
Since $cw > 0$, as $t > 0$ goes to infinity the objective function $cx(t)$ also tends to infinity, contradicting the fact that it is bounded above. Therefore, some $w$ satisfying Conditions (1) and (2) above must exist.

We show that there is some $t_0 > 0$ such that $cx(t_0) \geq cx_0$ and $x(t_0) = \tilde{x} + t_0w$ is feasible, yet $x(t_0)$ has more zero coordinates than $\tilde{x}$, a contradiction.

Since $x(t) = \tilde{x} + tw$, we have

$$x(t)_i = \tilde{x}_i + tw_i,$$

so if we let $I = \{i \in \{1, \ldots, n\} \mid w_i < 0\} \subseteq K$, which is nonempty since $w$ satisfies Condition (2) above, if we pick

$$t_0 = \min_{i \in I} \left\{ \frac{-\tilde{x}_i}{w_i} \right\},$$

then $t_0 > 0$, because $w_i < 0$ for all $i \in I$, and by definition of $K$ we have $\tilde{x}_i > 0$ for all $i \in K$. By the definition of $t_0 > 0$ and since $\tilde{x} \geq 0$, we have

$$x(t_0)_j = \tilde{x}_j + t_0w_j \geq 0 \quad \text{for all } j \in K,$$

so $x(t_0) \geq 0$, and $x(t_0)_i = 0$ for some $i \in I$. Since $Ax(t_0) = b$ (for any $t$), $x(t_0)$ is a feasible solution,

$$cx(t_0) = c\tilde{x} + t_0cw \geq cx_0 + t_0cw \geq cx_0,$$

and $x(t_0)_i = 0$ for some $i \in I$, we see that $x(t_0)$ has more zero coordinates than $\tilde{x}$, a contradiction. \qed

Proposition 26.3 implies the following important result.

**Theorem 9.4.** Let $(P_2)$ be any standard linear program with objective function $cx$, where $Ax = b$ and $A$ is an $m \times n$ matrix of rank $m$. If $(P_2)$ has some feasible solution and if it is bounded above, then some basic feasible solution $\tilde{x}$ is an optimal solution of $(P_2)$.

**Proof.** By Proposition 26.3, for any feasible solution $x$ there is some basic feasible solution $\tilde{x}$ such that $cx \leq c\tilde{x}$. But there are only finitely many basic feasible solutions, so one of them has to yield the maximum of the objective function. \qed

Geometrically, basic solutions are exactly the vertices of the polyhedron $P(A, b)$, a notion that we now define.

**Definition 9.6.** Given an $H$-polyhedron $P \subseteq \mathbb{R}^n$, a vertex of $P$ is a point $v \in P$ with property that there is some nonzero linear form $c \in (\mathbb{R}^n)^*$ and some $\mu \in \mathbb{R}$, such that $v$ is the unique point of $P$ for which the map $x \mapsto cx$ has the maximum value $\mu$; that is, $cy < cv = \mu$ for all $y \in P - \{v\}$. Geometrically this means that the hyperplane of equation $cy = \mu$ touches $P$ exactly at $v$. More generally, a convex subset $F$ of $P$ is a $k$-dimensional face of $P$ if $F$ has dimension $k$ and if there is some affine form $\varphi(x) = cx - \mu$ such that $cy = \mu$ for all $y \in F$, and $cy < \mu$ for all $y \in P - F$. A 1-dimensional face is called an edge.
9.2. BASIC FEASIBLE SOLUTIONS AND VERTICES

Figure 9.4: The cube centered at the origin with diagonal through \((-1, -1, -1)\) and \((1, 1, 1)\) has eight vertices. The vertex \((1, 1, 1)\) is associated with the linear form \(x + y + z = 3\).

The concept of a vertex is illustrated in Figure 26.4, while the concept of an edge is illustrated in Figure 26.5.

Since a \(k\)-dimensional face \(F\) of \(\mathcal{P}\) is equal to the intersection of the hyperplane \(H(\varphi)\) of equation \(cx = \mu\) with \(\mathcal{P}\), it is indeed convex and the notion of dimension makes sense. Observe that a 0-dimensional face of \(\mathcal{P}\) is a vertex. If \(\mathcal{P}\) has dimension \(d\), then the \((d - 1)\)-dimensional faces of \(\mathcal{P}\) are called its facets.

If \((P)\) is a linear program in standard form, then its basic feasible solutions are exactly the vertices of the polyhedron \(\mathcal{P}(A, b)\). To prove this fact we need the following simple proposition

**Proposition 9.5.** Let \(Ax = b\) be a linear system where \(A\) is an \(m \times n\) matrix of rank \(m\). For any subset \(K \subseteq \{1, \ldots, n\}\) of size \(m\), if \(A_K\) is invertible, then there is at most one basic feasible solution \(x \in \mathbb{R}^n\) with \(x_j = 0\) for all \(j /\in K\) (of course, \(x \geq 0\))

**Proof.** In order for \(x\) to be feasible we must have \(Ax = b\). Write \(N = \{1, \ldots, n\} - K\), \(x_K\) for the vector consisting of the coordinates of \(x\) with indices in \(K\), and \(x_N\) for the vector consisting of the coordinates of \(x\) with indices in \(N\). Then

\[Ax = A_Kx_K + A_Nx_N = b.\]

In order for \(x\) to be a basic feasible solution we must have \(x_N = 0\), so

\[A_Kx_K = b.\]

Since by hypothesis \(A_K\) is invertible, \(x_K = A_K^{-1}b\) is uniquely determined. If \(x_K \geq 0\) then \(x\) is a basic feasible solution, otherwise it is not. This proves that there is at most one basic feasible solution \(x \in \mathbb{R}^n\) with \(x_j = 0\) for all \(j /\in K\). \(\square\)
Figure 9.5: The cube centered at the origin with diagonal through $(-1, -1, -1)$ and $(1, 1, 1)$ has twelve edges. The vertex edge from $(1, 1, -1)$ to $(1, 1, 1)$ is associated with the linear form $x + y = 2$.

**Theorem 9.6.** Let $(P)$ be a linear program in standard form, where $Ax = b$ and $A$ is an $m \times n$ matrix of rank $m$. For every $v \in \mathcal{P}(A,b)$, the following conditions are equivalent:

1. $v$ is a vertex of the polyhedron $\mathcal{P}(A,b)$.

2. $v$ is a basic feasible solution of the linear program $(P)$.

**Proof.** First, assume that $v$ is a vertex of $\mathcal{P}(A,b)$, and let $\varphi(x) = cx - \mu$ be a linear form such that $cy < \mu$ for all $y \in \mathcal{P}(A,b)$ and $cv = \mu$. This means that $v$ is the unique point of $\mathcal{P}(A,b)$ for which the objective function $x \mapsto cx$ has the maximum value $\mu$ on $\mathcal{P}(A,b)$, so by Theorem 26.4, since this maximum is achieved by some basic feasible solution, by uniqueness $v$ must be a basic feasible solution.

Conversely, suppose $v$ is a basic feasible solution of $(P)$ corresponding to a subset $K \subseteq \{1, \ldots, n\}$ of size $m$. Let $\hat{c} \in (\mathbb{R}^n)^*$ be the linear form defined by

$$
\hat{c}_j = \begin{cases} 
0 & \text{if } j \in K \\
-1 & \text{if } j \notin K.
\end{cases}
$$

By construction $\hat{c}v = 0$ and $\hat{c}x \leq 0$ for any $x \geq 0$, hence the function $x \mapsto \hat{c}x$ on $\mathcal{P}(A,B)$ has a maximum at $v$. Furthermore, $\hat{c}x < 0$ for any $x \geq 0$ such that $x_j > 0$ for some $j \notin K$. However, by Proposition 26.5, the vector $v$ is the only basic feasible solution such that $v_j = 0$ for all $j \notin K$, and therefore $v$ is the only point of $\mathcal{P}(A,b)$ maximizing the function $x \mapsto \hat{c}x$, so it is a vertex. \hfill \Box
In theory, to find an optimal solution we try all \( \binom{n}{m} \) possible \( m \)-elements subsets \( K \) of \( \{1, \ldots, n\} \) and solve for the corresponding unique solution \( x_K \) of \( A_K x = b \). Then we check whether such a solution satisfies \( x_K \geq 0 \), compute \( cx_K \), and return some feasible \( x_K \) for which the objective function is maximum. This is a totally impracticable algorithm.

A practical algorithm is the simplex algorithm. Basically, the simplex algorithm tries to “climb” in the polyhedron \( P(A, b) \) from vertex to vertex along edges (using basic feasible solutions), trying to maximize the objective function. We present the simplex algorithm in the next chapter. The reader may also consult texts on linear programming. In particular, we recommend Matousek and Gardner [73], Chvatal [29], Papadimitriou and Steiglitz [80], Bertsimas and Tsitsiklis [17], Ciarlet [30], Schrijver [89], and Vanderbei [110].

Observe that Theorem 26.4 asserts that if a linear program \( (P) \) in standard form (where \( Ax = b \) and \( A \) is an \( m \times n \) matrix of rank \( m \)) has some feasible solution and is bounded above, then some basic feasible solution is an optimal solution. By Theorem 26.6, the polyhedron \( P(A, b) \) must have some vertex.

But suppose we only know that \( P(A, b) \) is nonempty; that is, we don’t know that the objective function \( cx \) is bounded above. Does \( P(A, b) \) have some vertex?

The answer to the above question is yes, and this is important because the simplex algorithm needs an initial basic feasible solution to get started. Here we prove that if \( P(A, b) \) is nonempty, then it must contain a vertex. This proof still doesn’t constructively yield a vertex, but we will see in the next chapter that the simplex algorithm always finds a vertex if there is one (provided that we use a pivot rule that prevents cycling).

**Theorem 9.7.** Let \( (P) \) be a linear program in standard form, where \( Ax = b \) and \( A \) is an \( m \times n \) matrix of rank \( m \). If \( P(A, b) \) is nonempty (there is a feasible solution), then \( P(A, b) \) has some vertex; equivalently, \( (P) \) has some basic feasible solution.

**Proof.** The proof relies on a trick, which is to add slack variables \( x_{n+1}, \ldots, x_{n+m} \) and use the new objective function \(- (x_{n+1} + \cdots + x_{n+m})\).

If we let \( \tilde{A} \) be the \( m \times (m+n) \)-matrix, and \( x, \overline{x}, \) and \( \hat{x} \) be the vectors given by

\[
\tilde{A} = \begin{pmatrix} A & I_m \end{pmatrix}, \quad x = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} \in \mathbb{R}^n, \quad \overline{x} = \begin{pmatrix} x_{n+1} \\ \vdots \\ x_{n+m} \end{pmatrix} \in \mathbb{R}^m, \quad \hat{x} = \begin{pmatrix} x \\ \overline{x} \end{pmatrix} \in \mathbb{R}^{n+m},
\]

then consider the linear program \( (\tilde{P}) \) in standard form

\[
\text{maximize} \quad - (x_{n+1} + \cdots + x_{n+m}) \\
\text{subject to} \quad \tilde{A} \hat{x} = b \text{ and } \hat{x} \geq 0.
\]

Since \( x_i \geq 0 \) for all \( i \), the objective function \(- (x_{n+1} + \cdots + x_{n+m}) \) is bounded above by 0. The system \( \tilde{A} \hat{x} = b \) is equivalent to the system

\[
Ax + \overline{x} = b,
\]
so for every feasible solution \( u \in \mathcal{P}(A,b) \), since \( Au = b \), the vector \((u,0)\) is also a feasible solution of \((\hat{P})\), in fact an optimal solution since the value of the objective function \(-\left(x_{n+1} + \cdots + x_{n+m}\right)\) for \( \bar{x} = 0 \) is 0. By Proposition 26.3, the linear program \((\hat{P})\) has some basic feasible solution \((u^*,w^*)\) for which the value of the objective function is greater than or equal to the value of the objective function for \((u,0)\), and since \((u,0)\) is an optimal solution, \((u^*,w^*)\) is also an optimal solution of \((\hat{P})\). This implies that \( w^* = 0 \), since otherwise the objective function \(-\left(x_{n+1} + \cdots + x_{n+m}\right)\) would have a strictly negative value.

Therefore, \((u^*,0)\) is a basic feasible solution of \((\hat{P})\), and thus the columns corresponding to nonzero components of \( u^* \) are linearly independent. Some of the coordinates of \( u^* \) could be equal to 0, but since \( A \) has rank \( m \) we can add columns of \( A \) to obtain a basis \( K \) associated with \( u^* \), and \( u^* \) is indeed a basic feasible solution of \((P)\).

The definition of a basic feasible solution can be adapted to linear programs where the constraints are of the form \( Ax \leq b, \ x \geq 0 \); see Matousek and Gardner [73] (Chapter 4, Section 4, Definition 4.4.2).

The most general type of linear program allows constraints of the form \( a_i x \geq b_i \) or \( a_i x = b_i \) besides constraints of the form \( a_i x \leq b_i \). The variables \( x_i \) may also take negative values. It is always possible to convert such programs to the type considered in Definition 26.1. We proceed as follows.

Every constraint \( a_i x \geq b_i \) is replaced by the constraint \(-a_i x \leq -b_i\). Every equality constraint \( a_i x = b_i \) is replaced by the two constraints \( a_i x \leq b_i \) and \(-a_i x \leq -b_i\).

If there are \( n \) variables \( x_i \), we create \( n \) new variables \( y_i \) and \( n \) new variables \( z_i \) and replace every variable \( x_i \) by \( y_i - z_i \). We also add the \( 2n \) constraints \( y_i \geq 0 \) and \( z_i \geq 0 \). If the constraints are given by the inequalities \( Ax \leq b \), we now have constraints given by

\[
\begin{pmatrix}
A & -A
\end{pmatrix}
\begin{pmatrix}
y \\
z
\end{pmatrix} \leq b,
\quad y \geq 0, \ z \geq 0.
\]

We replace the objective function \( cx \) by \( cy - cz \).

**Remark:** We also showed that we can replace the inequality constraints \( Ax \leq b \) by equality constraints \( Ax = b \), by adding slack variables constrained to be nonnegative.
Chapter 10

The Simplex Algorithm

10.1 The Idea Behind the Simplex Algorithm

The simplex algorithm, due to Dantzig, applies to a linear program \((P)\) in standard form, where the constraints are given by \(Ax = b\) and \(x \geq 0\), with \(A\) a \(m \times n\) matrix of rank \(m\), and with an objective function \(c \mapsto cx\). This algorithm either reports that \((P)\) has no feasible solution, or that \((P)\) is unbounded, or yields an optimal solution. Geometrically, the algorithm climbs from vertex to vertex in the polyhedron \(\mathcal{P}(A,b)\), trying to improve the value of the objective function. Since vertices correspond to basic feasible solutions, the simplex algorithm actually works with basic feasible solutions.

Recall that a basic feasible solution \(x\) is a feasible solution for which there is a subset \(K \subseteq \{1, \ldots, n\}\) of size \(m\) such that the matrix \(A_K\) consisting of the columns of \(A\) whose indices belong to \(K\) are linearly independent, and that \(x_j = 0\) for all \(j \notin K\). We also let \(J_>(x)\) be the set of indices

\[ J_>(x) = \{ j \in \{1, \ldots, n\} \mid x_j > 0 \}, \]

so for a basic feasible solution \(x\) associated with \(K\), we have \(J_>(x) \subseteq K\). In fact, by Proposition 26.2, a feasible solution \(x\) is a basic feasible solution iff the columns of \(A_{J_>(x)}\) are linearly independent.

If \(J_>(x)\) had cardinality \(m\) for all basic feasible solutions \(x\), then the simplex algorithm would make progress at every step, in the sense that it would strictly increase the value of the objective function. Unfortunately, it is possible that \(|J_>(x)| < m\) for certain basic feasible solutions, and in this case a step of the simplex algorithm may not increase the value of the objective function. Worse, in rare cases, it is possible that the algorithm enters an infinite loop. This phenomenon called cycling can be detected, but in this case the algorithm fails to give a conclusive answer.

Fortunately, there are ways of preventing the simplex algorithm from cycling (for example, Bland’s rule discussed later), although proving that these rules work correctly is quite involved.
The potential “bad” behavior of a basic feasible solution is recorded in the following definition.

**Definition 10.1.** Given a linear program \((P)\) in standard form where the constraints are given by \(Ax = b\) and \(x \geq 0\), with \(A\) an \(m \times n\) matrix of rank \(m\), a basic feasible solution \(x\) is *degenerate* if \(|J_{\geq}(x)| < m\), otherwise it is *nondegenerate*.

The origin \(0_n\), if it is a basic feasible solution, is degenerate. For a less trivial example, \(x = (0, 0, 0, 2)\) is a degenerate basic feasible solution of the following linear program in which \(m = 2\) and \(n = 4\).

**Example 10.1.**

\[
\begin{align*}
\text{maximize} & \quad x_2 \\
\text{subject to} & \quad -x_1 + x_2 + x_3 = 0 \\
& \quad x_1 + x_4 = 2 \\
& \quad x_1 \geq 0, \ x_2 \geq 0, \ x_3 \geq 0, \ x_4 \geq 0.
\end{align*}
\]

The matrix \(A\) and the vector \(b\) are given by
\[
A = \begin{pmatrix}
-1 & 1 & 1 & 0 \\
1 & 0 & 0 & 1
\end{pmatrix}, \quad b = \begin{pmatrix}
0 \\
2
\end{pmatrix},
\]
and if \(x = (0, 0, 0, 2)\), then \(J_{\geq}(x) = \{4\}\). There are two ways of forming a set of two linearly independent columns of \(A\) containing the fourth column.

Given a basic feasible solution \(x\) associated with a subset \(K\) of size \(m\), since the columns of the matrix \(A_K\) are linearly independent, by abuse of language we call the columns of \(A_K\) a *basis* of \(x\).

If \(u\) is a vertex of \((P)\), that is, a basic feasible solution of \((P)\) associated with a basis \(K\) (of size \(m\)), in “normal mode,” the simplex algorithm tries to move along an edge from the vertex \(u\) to an adjacent vertex \(v\) (with \(u, v \in \mathcal{P}(A,b) \subseteq \mathbb{R}^n\)) corresponding to a basic feasible solution whose basis is obtained by replacing one of the basic vectors \(A_k\) with \(k \in K\) by another nonbasic vector \(A_j\) for some \(j \notin K\), in such a way that the value of the objective function is increased.

Let us demonstrate this process on an example.

**Example 10.2.** Let \((P)\) be the following linear program in standard form.

\[
\begin{align*}
\text{maximize} & \quad x_1 + x_2 \\
\text{subject to} & \quad -x_1 + x_2 + x_3 = 1 \\
& \quad x_1 + x_4 = 3 \\
& \quad x_2 + x_5 = 2 \\
& \quad x_1 \geq 0, \ x_2 \geq 0, \ x_3 \geq 0, \ x_4 \geq 0, \ x_5 \geq 0.
\end{align*}
\]
The matrix $A$ and the vector $b$ are given by

$$
A = \begin{pmatrix}
-1 & 1 & 1 & 0 & 0 \\
1 & 0 & 0 & 1 & 0 \\
0 & 1 & 0 & 0 & 1
\end{pmatrix}, \quad b = \begin{pmatrix}
1 \\
3 \\
2
\end{pmatrix}.
$$

Figure 10.1: The planar $\mathcal{H}$-polyhedron associated with Example 27.2. The initial basic feasible solution is the origin. The simplex algorithm first moves along the horizontal orange line to feasible solution at vertex $u_1$. It then moves along the vertical red line to obtain the optimal feasible solution $u_2$.

The vector $u_0 = (0, 0, 1, 3, 2)$ corresponding to the basis $K = \{3, 4, 5\}$ is a basic feasible solution, and the corresponding value of the objective function is $0 + 0 = 0$. Since the columns $(A^3, A^4, A^5)$ corresponding to $K = \{3, 4, 5\}$ are linearly independent we can express $A^1$ and $A^2$ as

$$
A^1 = -A^3 + A^4 \\
A^2 = A^3 + A^5.
$$

Since

$$
1A^3 + 3A^4 + 2A^5 = Au_0 = b,
$$

for any $\theta \in \mathbb{R}$, we have

$$
b = 1A^3 + 3A^4 + 2A^5 - \theta A^1 + \theta A^1 \\
= 1A^3 + 3A^4 + 2A^5 - \theta(-A^3 + A^4) + \theta A^1 \\
= \theta A^1 + (1 + \theta)A^3 + (3 - \theta)A^4 + 2A^5,
$$
and

\[ b = 1A^3 + 3A^4 + 2A^5 - \theta A^2 + \theta A^2 \]
\[ = 1A^3 + 3A^4 + 2A^5 - \theta(A^3 + A^5) + \theta A^1 \]
\[ = \theta A^2 + (1 - \theta)A^3 + 3A^4 + (2 - \theta)A^5. \]

In the first case, the vector \((\theta, 0, 1 + \theta, 3 - \theta, 2)\) is a feasible solution iff \(0 \leq \theta \leq 3\), and the new value of the objective function is \(\theta\).

In the second case, the vector \((0, \theta, 1 - \theta, 3, 2 - \theta, 1)\) is a feasible solution iff \(0 \leq \theta \leq 1\), and the new value of the objective function is also \(\theta\).

Consider the first case. It is natural to ask whether we can get another vertex and increase the objective function by setting to zero one of the coordinates of \((\theta, 0, 1 + \theta, 3 - \theta, 2)\), in this case the fourth one, by picking \(\theta = 3\). This yields the feasible solution \((3, 0, 4, 0, 2)\), which corresponds to the basis \((A^1, A^3, A^5)\), and so is indeed a basic feasible solution, with an improved value of the objective function equal to 3. Note that \(A^4\) left the basis \((A^3, A^4, A^5)\) and \(A^1\) entered the new basis \((A^1, A^3, A^5)\).

We can now express \(A^2\) and \(A^4\) in terms of the basis \((A^1, A^3, A^5)\), which is easy to do since we already have \(A^1\) and \(A^2\) in term of \((A^3, A^4, A^5)\), and \(A^1\) and \(A^4\) are swapped. Such a step is called a \textit{pivoting step}. We obtain

\[ A^2 = A^3 + A^5 \]
\[ A^4 = A^1 + A^3. \]

Then we repeat the process with \(u_1 = (3, 0, 4, 0, 2)\) and the basis \((A^1, A^3, A^5)\). We have

\[ b = 3A^1 + 4A^3 + 2A^5 - \theta A^2 + \theta A^2 \]
\[ = 3A^1 + 4A^3 + 2A^5 - \theta(A^3 + A^5) + \theta A^2 \]
\[ = 3A^1 + \theta A^2 + (4 - \theta)A^3 + (2 - \theta)A^5, \]
and

\[ b = 3A^1 + 4A^3 + 2A^5 - \theta A^4 + \theta A^4 \]
\[ = 3A^1 + 4A^3 + 2A^5 - \theta(A^1 + A^5) + \theta A^4 \]
\[ = (3 - \theta)A^1 + (4 - \theta)A^3 + \theta A^4 + 2A^5. \]

In the first case, the point \((3, \theta, 4 - \theta, 0, 2 - \theta)\) is a feasible solution iff \(0 \leq \theta \leq 2\), and the new value of the objective function is \(3 + \theta\). In the second case, the point \((3 - \theta, 0, 4 - \theta, \theta, 2)\) is a feasible solution iff \(0 \leq \theta \leq 3\), and the new value of the objective function is \(3 - \theta\). To increase the objective function we must choose the first case and we pick \(\theta = 2\). Then, we get the feasible solution \(u_2 = (3, 2, 2, 0, 0)\), which corresponds to the basis \((A^1, A^2, A^3)\), and thus is a basic feasible solution. The new value of the objective function is 5.
10.1. THE IDEA BEHIND THE SIMPLEX ALGORITHM

Next we express $A^4$ and $A^5$ in terms of the basis $(A^1, A^2, A^3)$. Again this is easy to do since we just swapped $A^5$ and $A^2$ (a pivoting step), and we get

\[
A^5 = A^2 - A^3 \\
A^4 = A^1 + A^3.
\]

We repeat the process with $u_2 = (3, 2, 2, 0, 0)$ and the basis $(A^1, A^2, A^3)$. We have

\[
b = 3A^1 + 2A^2 + 2A^3 - \theta A^4 + \theta A^4 \\
= 3A^1 + 2A^2 + 2A^3 - \theta(A^1 + A^3) + \theta A^4 \\
= (3 - \theta)A^1 + 2A^2 + (2 - \theta)A^3 + \theta A^4,
\]

and

\[
b = 3A^1 + 2A^2 + 2A^3 - \theta A^5 + \theta A^5 \\
= 3A^1 + 2A^2 + 2A^3 - \theta(A^2 - A^3) + \theta A^5 \\
= 3A^1 + (2 - \theta)A^2 + (2 + \theta)A^3 + \theta A^5.
\]

In the first case, the point $(3 - \theta, 2, 2 - \theta, \theta, 0)$ is a feasible solution iff $0 \leq \theta \leq 2$, and the value of the objective function is $5 - \theta$. In the second case, the point $(3, 2 - \theta, 2 + \theta, 0, \theta)$ is a feasible solution iff $0 \leq \theta \leq 2$, and the value of the objective function is also $5 - \theta$. Since we must have $\theta \geq 0$ to have a feasible solution, there is no way to increase the objective function. In this situation, it turns out that we have reached an optimal solution, in our case $u_2 = (3, 2, 2, 0, 0)$, with the maximum of the objective function equal to 5.

We could also have applied the simplex algorithm to the vertex $u_0 = (0, 0, 1, 3, 2)$ and to the vector $(0, \theta, 1 - \theta, 3, 2 - \theta, 1)$, which is a feasible solution iff $0 \leq \theta \leq 1$, with new value of the objective function $\theta$. By picking $\theta = 1$, we obtain the feasible solution $(0, 1, 0, 3, 1)$, corresponding to the basis $(A^2, A^4, A^5)$, which is indeed a vertex. The new value of the objective function is 1. Then we express $A^1$ and $A^3$ in terms the basis $(A^2, A^4, A^5)$ obtaining

\[
A^1 = A^4 - A^3 \\
A^3 = A^2 - A^5,
\]

and repeat the process with $(0, 1, 0, 3, 1)$ and the basis $(A^2, A^4, A^5)$. After three more steps we will reach the optimal solution $u_2 = (3, 2, 2, 0, 0)$.

Let us go back to the linear program of Example 27.1 with objective function $x_2$ and where the matrix $A$ and the vector $b$ are given by

\[
A = \begin{pmatrix} -1 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix}, \quad b = \begin{pmatrix} 0 \\ 2 \end{pmatrix}.
\]

Recall that $u_0 = (0, 0, 0, 2)$ is a degenerate basic feasible solution, and the objective function has the value 0. See Figure 27.2 for a planar picture of the $H$-polyhedron associated with Example 27.1.
Figure 10.2: The planar $H$-polyhedron associated with Example 27.1. The initial basic feasible solution is the origin. The simplex algorithm moves along the slanted orange line to the apex of the triangle.

Pick the basis $(A^3, A^4)$. Then we have

$$A^1 = -A^3 + A^4$$
$$A^2 = A^3,$$

and we get

$$b = 2A^4 - \theta A^1 + \theta A^1$$
$$= 2A^4 - \theta(-A^3 + A^4) + \theta A^1$$
$$= \theta A^1 + \theta A^3 + (2 - \theta)A^4,$$

and

$$b = 2A^4 - \theta A^2 + \theta A^2$$
$$= 2A^4 - \theta A^3 + \theta A^2$$
$$= \theta A^2 - \theta A^3 + 2A^4.$$

In the first case, the point $(\theta, 0, \theta, 2 - \theta)$ is a feasible solution iff $0 \leq \theta \leq 2$, and the value of the objective function is 0, and in the second case the point $(0, \theta, -\theta, 2)$ is a feasible solution iff $\theta = 0$, and the value of the objective function is $\theta$. However, since we must have $\theta = 0$ in the second case, there is no way to increase the objective function either.

It turns out that in order to make the cases considered by the simplex algorithm as mutually exclusive as possible, since in the second case the coefficient of $\theta$ in the value of the objective function is nonzero, namely 1, we should choose the second case. We must
pick $\theta = 0$, but we can swap the vectors $A^3$ and $A^2$ (because $A^2$ is coming in and $A^3$ has the coefficient $-\theta$, which is the reason why $\theta$ must be zero), and we obtain the basic feasible solution $u_1 = (0,0,0,2)$ with the new basis $(A^2,A^4)$. Note that this basic feasible solution corresponds to the same vertex $(0,0,0,2)$ as before, but the basis has changed. The vectors $A^1$ and $A^3$ can be expressed in terms of the basis $(A^2,A^4)$ as

$$A^1 = -A^2 + A^4$$
$$A^3 = A^2.$$

We now repeat the procedure with $u_1 = (0,0,0,2)$ and the basis $(A^2,A^4)$, and we get

$$b = 2A^4 - \theta A^1 + \theta A^3$$
$$= 2A^4 - \theta(-A^2 + A^4) + \theta A^1$$
$$= \theta A^1 + \theta A^2 + (2 - \theta)A^4,$$

and

$$b = 2A^4 - \theta A^3 + \theta A^3$$
$$= 2A^4 - \theta A^2 + \theta A^3$$
$$= -\theta A^2 + \theta A^3 + 2A^4.$$

In the first case, the point $(\theta,\theta,0,2-\theta)$ is a feasible solution iff $0 \leq \theta \leq 2$ and the value of the objective function is $\theta$, and in the second case the point $(0,-\theta,\theta,2)$ is a feasible solution iff $\theta = 0$ and the value of the objective function is $\theta$. In order to increase the objective function we must choose the first case and pick $\theta = 2$. We obtain the feasible solution $u_2 = (2,2,0,0)$ whose corresponding basis is $(A^1,A^2)$ and the value of the objective function is 2.

The vectors $A^3$ and $A^4$ are expressed in terms of the basis $(A^1,A^2)$ as

$$A^3 = A^2$$
$$A^4 = A^1 + A^3,$$

and we repeat the procedure with $u_2 = (2,2,0,0)$ and the basis $(A^1,A^2)$. We get

$$b = 2A^1 + 2A^2 - \theta A^3 + \theta A^3$$
$$= 2A^1 + 2A^2 - \theta A^2 + \theta A^3$$
$$= 2A^1 + (2 - \theta)A^2 + \theta A^3,$$

and

$$b = 2A^1 + 2A^2 - \theta A^4 + \theta A^4$$
$$= 2A^1 + 2A^2 - \theta(A^1 + A^3) + \theta A^4$$
$$= (2 - \theta)A^1 + 2A^2 - \theta A^3 + \theta A^4.$$
In the first case, the point \((2, 2 - \theta, 0, \theta)\) is a feasible solution iff \(0 \leq \theta \leq 2\) and the value of the objective function is \(2 - \theta\), and in the second case, the point \((2 - \theta, 2, -\theta, \theta)\) is a feasible solution iff \(\theta = 0\) and the value of the objective function is 2. This time there is no way to improve the objective function and we have reached an optimal solution \(u_2 = (2, 2, 0, 0)\) with the maximum of the objective function equal to 2.

Let us now consider an example of an unbounded linear program.

**Example 10.3.** Let \((P)\) be the following linear program in standard form.

\[
\begin{align*}
\text{maximize} & \quad x_1 \\
\text{subject to} & \quad x_1 - x_2 + x_3 = 1 \\
& \quad -x_1 + x_2 + x_4 = 2 \\
& \quad x_1 \geq 0, \ x_2 \geq 0, \ x_3 \geq 0, \ x_4 \geq 0.
\end{align*}
\]

The matrix \(A\) and the vector \(b\) are given by

\[
A = \begin{pmatrix}
1 & -1 & 1 & 0 \\
-1 & 1 & 0 & 1
\end{pmatrix}, \quad b = \begin{pmatrix}
1 \\
2
\end{pmatrix}.
\]

Figure 10.3: The planar \(\mathcal{H}\)-polyhedron associated with Example 27.3. The initial basic feasible solution is the origin. The simplex algorithm first moves along the horizontal indigo line to basic feasible solution at vertex \((1, 0)\). Any optimal feasible solution occurs by moving along the boundary line parameterized by the orange arrow \(\theta(1, 1)\).

The vector \(u_0 = (0, 0, 1, 2)\) corresponding to the basis \(K = \{3, 4\}\) is a basic feasible solution, and the corresponding value of the objective function is 0. The vectors \(A^1\) and \(A^2\)
are expressed in terms of the basis \((A^3, A^4)\) by
\[
\begin{align*}
A^1 &= A^3 - A^4 \\
\end{align*}
\]
Starting with \(u_0 = (0, 0, 1, 2)\), we get
\[
\begin{align*}
b &= A^3 + 2A^4 - \theta A^1 + \theta A^1 \\
&= A^3 + 2A^4 - \theta(A^3 - A^4) + \theta A^1 \\
&= \theta A^1 + (1 - \theta)A^3 + (2 + \theta)A^4,
\end{align*}
\]
and
\[
\begin{align*}
b &= A^3 + 2A^4 - \theta A^2 + \theta A^2 \\
&= A^3 + 2A^4 - \theta(-A^3 + A^4) + \theta A^2 \\
&= \theta A^2 + (1 + \theta)A^3 + (2 - \theta)A^4.
\end{align*}
\]
In the first case, the point \((\theta, 0, 1 - \theta, 2 + \theta)\) is a feasible solution iff \(0 \leq \theta \leq 1\) and the value of the objective function is \(\theta\); and in the second case, the point \((0, \theta, 1 + \theta, 2 - \theta)\) is a feasible solution iff \(0 \leq \theta \leq 2\) and the value of the objective function is 0. In order to increase the objective function we must choose the first case, and we pick \(\theta = 1\). We get the feasible solution \(u_1 = (1, 0, 0, 3)\) corresponding to the basis \((A^1, A^4)\), so it is a basic feasible solution, and the value of the objective function is 1.

The vectors \(A^2\) and \(A^3\) are given in terms of the basis \((A^1, A^4)\) by
\[
\begin{align*}
A^2 &= -A^1 \\
A^3 &= A^1 + A^4.
\end{align*}
\]
Repeating the process with \(u_1 = (1, 0, 0, 3)\), we get
\[
\begin{align*}
b &= A^1 + 3A^4 - \theta A^2 + \theta A^2 \\
&= A^1 + 3A^4 - \theta(-A^1) + \theta A^2 \\
&= (1 + \theta)A^1 + \theta A^2 + 3A^4,
\end{align*}
\]
and
\[
\begin{align*}
b &= A^1 + 3A^4 - \theta A^3 + \theta A^3 \\
&= A^1 + 3A^4 - \theta(A^1 + A^4) + \theta A^3 \\
&= (1 - \theta)A^1 + \theta A^3 + (3 - \theta)A^4.
\end{align*}
\]
In the first case, the point \((1 + \theta, \theta, 0, 3)\) is a feasible solution for all \(\theta \geq 0\) and the value of the objective function if \(1 + \theta\), and in the second case, the point \((1 - \theta, 0, \theta, 3 - \theta)\) is a
feasible solution iff $0 \leq \theta \leq 1$ and the value of the objective function is $1 - \theta$. This time, we are in the situation where the points

$$(1 + \theta, \theta, 0, 3) = (1, 0, 0, 3) + \theta(1, 1, 0, 0), \quad \theta \geq 0$$

form an infinite ray in the set of feasible solutions, and the objective function $1 + \theta$ is unbounded from above on this ray. This indicates that our linear program, although feasible, is unbounded.

Let us now describe a step of the simplex algorithm in general.

### 10.2 The Simplex Algorithm in General

We assume that we already have an initial vertex $u_0$ to start from. This vertex corresponds to a basic feasible solution with basis $K_0$. We will show later that it is always possible to find a basic feasible solution of a linear program $(P)$ in standard form, or to detect that $(P)$ has no feasible solution.

The idea behind the simplex algorithm is this: Given a pair $(u, K)$ consisting of a basic feasible solution $u$ and a basis $K$ for $u$, find another pair $(u^+, K^+)$ consisting of another basic feasible solution $u^+$ and a basis $K^+$ for $u^+$, such that $K^+$ is obtained from $K$ by deleting some basic index $k^- \in K$ and adding some nonbasic index $j^+ \notin K$, in such a way that the value of the objective function increases (preferably strictly). The step which consists in swapping the vectors $A^{k^-}$ and $A^{j^+}$ is called a pivoting step.

Let $u$ be a given vertex corresponds to a basic feasible solution with basis $K$. Since the $m$ vectors $A^k$ corresponding to indices $k \in K$ are linearly independent, they form a basis, so for every nonbasic $j \notin K$, we write

$$A^j = \sum_{k \in K} \gamma^j_k A^k. \quad (*)$$

We let $\gamma^j_K \in \mathbb{R}^m$ be the vector given by $\gamma^j_k = (\gamma^j_k)_k \in K$. Actually, since the vector $\gamma^j_K$ depends on $K$, to be very precise we should denote its components by $(\gamma^j_K)_k$, but to simplify notation we usually write $\gamma^j_k$ instead of $(\gamma^j_K)_k$ (unless confusion arises). We will explain later how the coefficients $\gamma^j_k$ can be computed efficiently.

Since $u$ is a feasible solution we have $u \geq 0$ and $Au = b$, that is,

$$\sum_{k \in K} u_k A^k = b. \quad (**)$$

For every nonbasic $j \notin K$, a candidate for entering the basis $K$, we try to find a new vertex $u(\theta)$ that improves the objective function, and for this we add $-\theta A^j + \theta A^j = 0$ to $b$ in
the equation (***) and then replace the occurrence of \( A^j \) in \(-\theta A^j\) by the right hand side of equation (*) to obtain

\[
b = \sum_{k \in K} u_k A^k - \theta A^j + \theta A^j
\]

\[
= \sum_{k \in K} u_k A^k - \theta \left( \sum_{k \in K} \gamma_k^j A^k \right) + \theta A^j
\]

\[
= \sum_{k \in K} \left( u_k - \theta \gamma_k^j \right) A^k + \theta A^j.
\]

Consequently, the vector \( u(\theta) \) appearing on the right-hand side of the above equation given by

\[
u(\theta)_i = \begin{cases} u_i - \theta \gamma_i^j & \text{if } i \in K \\ \theta & \text{if } i = j \\ 0 & \text{if } i \notin K \cup \{j\} \end{cases}
\]

automatically satisfies the constraints \( Au(\theta) = b \), and this vector is a feasible solution iff

\[
\theta \geq 0 \quad \text{and} \quad u_k \geq \theta \gamma_k^j \quad \text{for all } k \in K.
\]

Obviously \( \theta = 0 \) is a solution, and if

\[
\theta^j = \min \left\{ \frac{u_k}{\gamma_k^j} \mid \gamma_k^j > 0, \ k \in K \right\} > 0,
\]

then we have a range of feasible solutions for \( 0 \leq \theta \leq \theta^j \). The value of the objective function for \( u(\theta) \) is

\[
cu(\theta) = \sum_{k \in K} c_k (u_k - \theta \gamma_k^j) + \theta c_j = cu + \theta \left( c_j - \sum_{k \in K} \gamma_k^j c_k \right).
\]

Since the potential change in the objective function is

\[
\theta \left( c_j - \sum_{k \in K} \gamma_k^j c_k \right)
\]

and \( \theta \geq 0 \), if \( c_j - \sum_{k \in K} \gamma_k^j c_k \leq 0 \) then the objective function can’t be increased.

However, if \( c_j^+ - \sum_{k \in K} \gamma_k^j c_k > 0 \) for some \( j^+ \notin K \), and if \( \theta^j > 0 \), then the objective function can be strictly increased by choosing any \( \theta > 0 \) such that \( \theta \leq \theta^j \), so it is natural to zero at least one coefficient of \( u(\theta) \) by picking \( \theta = \theta^j \), which also maximizes the increase of the objective function. In this case (Case below (B2)), we obtain a new feasible solution \( u^+ = u(\theta^j) \).

Now, if \( \theta^j > 0 \), then there is some index \( k \in K \) such \( u_k > 0 \), \( \gamma_k^j > 0 \), and \( \theta^j = u_k / \gamma_k^j \), so we can pick such an index \( k^- \) for the vector \( A^k^- \) leaving the basis \( K \). We claim that
$K^+ = (K - \{k^-\}) \cup \{j^+\}$ is a basis. This is because the coefficient $\gamma_{k^-}^j$ associated with the column $A_k^-$ is nonzero (in fact, $\gamma_{k^-}^j > 0$), so equation (*) yields

$$A_j^+ = \gamma_{k^-}^j A_k^- + \sum_{k \in K - \{k^-\}} \gamma_k^j A_k^-$$

yields the equation

$$A_k^- = (\gamma_{k^-}^j)^{-1} A_j^+ - \sum_{k \in K - \{k^-\}} (\gamma_{k^-}^j)^{-1} \gamma_k^j A_k^-$$

and these equations imply that the subspaces spanned by the vectors $(A^k)_{k \in K}$ and the vectors $(A^k)_{k \in K^+}$ are identical. However, $K$ is a basis of dimension $m$ so this subspace has dimension $m$, and since $K^+$ also has $m$ elements, it must be a basis. Therefore, $u^+ = u(\theta^{j^+})$ is a basic feasible solution.

The above case is the most common one, but other situations may arise. In what follows, we discuss all eventualities.

Case (A).

We have $c_j - \sum_{k \in K} \gamma_k^j c_k \leq 0$ for all $j \notin K$. Then it turns out that $u$ is an optimal solution. Otherwise, we are in Case (B).

Case (B).

We have $c_j - \sum_{k \in K} \gamma_k^j c_k > 0$ for some $j \notin K$ (not necessarily unique). There are three subcases.

Case (B1).

If for some $j \notin K$ as above we also have $\gamma_k^j \leq 0$ for all $k \in K$, since $u_k \geq 0$ for all $k \in K$, this places no restriction on $\theta$, and the objective function is unbounded above.

Case (B2).

There is some index $j^+ \notin K$ such that simultaneously

1. $c_{j^+} - \sum_{k \in K} \gamma_{k}^{j^+} c_k > 0$, which means that the objective function can potentially be increased;

2. There is some $k \in K$ such that $\gamma_k^{j^+} > 0$, and for every $k \in K$, if $\gamma_k^{j^+} > 0$ then $u_k > 0$, which implies that $\theta^{j^+} > 0$.

If we pick $\theta = \theta^{j^+}$ where

$$\theta^{j^+} = \min \left\{ \frac{u_k}{\gamma_k^{j^+}} \left| \gamma_k^{j^+} > 0, k \in K \right\} > 0,$$
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then the feasible solution \( u^+ \) given by

\[
u_i^+ = \begin{cases} 
  u_i - \theta_i^+ \gamma_i^+ & \text{if } i \in K \\
  \theta^+ & \text{if } i = j^+ \\
  0 & \text{if } i \notin K \cup \{j^+\}
\end{cases}
\]

is a vertex of \( \mathcal{P}(A,b) \). If we pick any index \( k^- \in K \) such that \( \theta_i^+ = u_{k^-} / \gamma_{k^-}^j \), then \( K^+ = (K - \{k^-\}) \cup \{j^+\} \) is a basis for \( u^+ \). The vector \( A^{j^+} \) enters the new basis \( K^+ \), and the vector \( A^{k^-} \) leaves the old basis \( K \). This is a pivoting step. The objective function increases strictly.

**Case (B3).**

There is some index \( j \notin K \) such that \( c_j - \sum_{k \in K} \gamma_k^j c_k > 0 \), and for each of the indices \( j \notin K \) satisfying the above property we have simultaneously

1. \( c_j - \sum_{k \in K} \gamma_k^j c_k > 0 \), which means that the objective function can potentially be increased;

2. There is some \( k \in K \) such that \( \gamma_k^j > 0 \), and \( u_k = 0 \), which implies that \( \theta_j^i = 0 \).

Consequently, the objective function does not change. In this case, \( u \) is a degenerate basic feasible solution.

We can associate to \( u^+ = u \) a new basis \( K^+ \) as follows: Pick any index \( j^+ \notin K \) such that

\[
c_{j^+} - \sum_{k \in K} \gamma_k^{j^+} c_k > 0,
\]

and any index \( k^- \in K \) such that

\[
\gamma_{k^-}^{j^+} > 0,
\]

and let \( K^+ = (K - \{k^-\}) \cup \{j^+\} \). As in Case (B2), The vector \( A^{j^+} \) enters the new basis \( K^+ \), and the vector \( A^{k^-} \) leaves the old basis \( K \). This is a pivoting step. However, the objective function does not change since \( \theta_i^+ = 0 \).

It is easy to prove that in Case (A) the basic feasible solution \( u \) is an optimal solution, and that in Case (B1) the linear program is unbounded. We already proved that in Case (B2) the vector \( u^+ \) and its basis \( K^+ \) constitutes a basic feasible solution, and the proof in Case (B3) is similar. For details, see Ciarlet [30] (Chapter 10).

It is convenient to reinterpret the various cases considered by introducing the followings sets:

\[
B_1 = \left\{ j \notin K \mid c_j - \sum_{k \in K} \gamma_k^j c_k > 0, \max_{k \in K} \gamma_k^j \leq 0 \right\}
\]

\[
B_2 = \left\{ j \notin K \mid c_j - \sum_{k \in K} \gamma_k^j c_k > 0, \max_{k \in K} \gamma_k^j > 0, \min \left\{ \frac{u_k}{\gamma_k^j} \mid k \in K, \gamma_k^j > 0 \right\} > 0 \right\}
\]

\[
B_3 = \left\{ j \notin K \mid c_j - \sum_{k \in K} \gamma_k^j c_k > 0, \max_{k \in K} \gamma_k^j > 0, \min \left\{ \frac{u_k}{\gamma_k^j} \mid k \in K, \gamma_k^j > 0 \right\} = 0 \right\},
\]
and
\[ B = B_1 \cup B_2 \cup B_3 = \left\{ j \notin K \mid c_j - \sum_{k \in K} \gamma^j_k c_k > 0 \right\}. \]

Then it is easy to see that the following equivalences hold:

- Case (A) \iff B = \emptyset,
- Case (B) \iff B \neq \emptyset
- Case (B1) \iff B_1 \neq \emptyset
- Case (B2) \iff B_2 \neq \emptyset
- Case (B3) \iff B_3 \neq \emptyset.

Furthermore, (A) and (B), (B1) and (B3), (B2) and (B3) are mutually exclusive, while (B1) and (B2) are not.

If Case (B1) and Case (B2) arise simultaneously, we opt for Case (B1) which says that the linear program \((P)\) is unbounded and terminate the algorithm.

Here are a few remarks about the method.

In Case (B2), which is the path followed by the algorithm most frequently, various choices have to be made for the index \(j^+ \notin K\) for which \(\theta^j > 0\) (the new index in \(K^+\)). Similarly, various choices have to be made for the index \(k^- \in K\) leaving \(K\), but such choices are typically less important.

Similarly in Case (B3), various choices have to be made for the new index \(j^+ \notin K\) going into \(K^+\). In Cases (B2) and (B3), criteria for making such choices are called **pivot rules**.

Case (B3) only arises when \(u\) is a degenerate vertex. But even if \(u\) is degenerate, Case (B2) may arise if \(u_k > 0\) whenever \(\gamma^j_k > 0\). It may also happen that \(u\) is nondegenerate but as a result of Case (B2), the new vertex \(u^+\) is degenerate because at least two components \(u_{k_1} - \theta^j \gamma^j_{k_1}\) and \(u_{k_2} - \theta^j \gamma^j_{k_2}\) vanish for some distinct \(k_1, k_2 \in K\).

Cases (A) and (B1) correspond to situations where the algorithm terminates, and Case (B2) can only arise a finite number of times during execution of the simplex algorithm, since the objective function is strictly increased from vertex to vertex and there are only finitely many vertices. Therefore, if the simplex algorithm is started on any initial basic feasible solution \(u_0\), then one of three mutually exclusive situations may arise:

1. There is a finite sequence of occurrences of Case (B2) and/or Case (B3) ending with an occurrence of Case (A). Then the last vertex produced by the algorithm is an optimal solution.

2. There is a finite sequence of occurrences of Case (B2) and/or Case (B3) ending with an occurrence of Case (B1). We conclude that the problem is unbounded, and thus has no solution.
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(3) There is a finite sequence of occurrences of Case (B2) and/or Case (B3), followed by an infinite sequence of Case (B3). If this occurs, the algorithm visits the same basis twice. This a phenomenon known as cycling. In this eventually the algorithm fails to come to a conclusion.

There are examples for which cycling occur, although this is rare in practice. Such an example is given in Chvatal [29]; see Chapter 3, pages 31-32, for an example with seven variables and three equations that cycles after six iterations under a certain pivot rule.

The third possibility can be avoided by the choice of a suitable pivot rule. Two of these rules are Bland’s rule and the lexicographic rule; see Chvatal [29] (Chapter 3, pages 34-38).

Bland’s rule says: choose the smallest of the eligible incoming indices \( j^+ \notin K \), and similarly choose the smallest of the eligible outgoing indices \( k^- \in K \).

It can be proved that cycling cannot occur if Bland’s rule is chosen as the pivot rule. The proof is very technical; see Chvatal [29] (Chapter 3, pages 37-38), Matousek and Gardner [73] (Chapter 5, Theorem 5.8.1), and Papadimitriou and Steiglitz [80] (Section 2.7). Therefore, assuming that some initial basic feasible solution is provided, and using a suitable pivot rule (such as Bland’s rule), the simplex algorithm always terminates and either yields an optimal solution or reports that the linear program is unbounded. Unfortunately Bland’s rules is one of the slowest pivot rules.

The choice of a pivot rule affects greatly the number of pivoting steps that the simplex algorithms goes through. It is not our intention here to explain the various pivot rules. We simply mention the following rules, referring the reader to Matousek and Gardner [73] (Chapter 5, Section 5.7) or to the texts cited in Section 25.1.

1. Largest coefficient.
2. Largest increase.
3. Steepest edge.
5. Random edge.

The steepest edge rule is one of the most popular. The idea is to maximize the ratio

\[
\frac{c(u^+ - u)}{\|u^+ - u\|}.
\]

The random edge rule picks the index \( j^+ \notin K \) of the entering basis vector uniformly at random among all eligible indices.

Let us now return to the issue of the initialization of the simplex algorithm. We use the linear program (\( \hat{P} \)) introduced during the proof of Theorem 26.7.
Consider a linear program (P2)

\[
\begin{align*}
\text{maximize} \quad & cx \\
\text{subject to} \quad & Ax = b \quad \text{and} \quad x \geq 0,
\end{align*}
\]

in standard form where \( A \) is an \( m \times n \) matrix of rank \( m \).

First, observe that since the constraints are equations, we can ensure that \( b \geq 0 \), because every equation \( a_i x = b_i \) where \( b_i < 0 \) can be replaced by \( -a_i x = -b_i \). The next step is to introduce the linear program (\( \hat{P} \)) in standard form

\[
\begin{align*}
\text{maximize} \quad & -(x_{n+1} + \cdots + x_{n+m}) \\
\text{subject to} \quad & \hat{A} \hat{x} = b \quad \text{and} \quad \hat{x} \geq 0,
\end{align*}
\]

where \( \hat{A} \) and \( \hat{x} \) are given by

\[
\hat{A} = (A \ I_m), \quad \hat{x} = \begin{pmatrix} x_1 \\ \vdots \\ x_{n+m} \end{pmatrix}.
\]

Since we assumed that \( b \geq 0 \), the vector \( \hat{x} = (0_n, b) \) is a feasible solution of (\( \hat{P} \)), in fact a basic feasible solutions since the matrix associated with the indices \( n+1, \ldots, n+m \) is the identity matrix \( I_m \). Furthermore, since \( x_i \geq 0 \) for all \( i \), the objective function \( -(x_{n+1} + \cdots + x_{n+m}) \) is bounded above by 0.

If we execute the simplex algorithm with a pivot rule that prevents cycling, starting with the basic feasible solution \( (0_n, d) \), since the objective function is bounded by 0, the simplex algorithm terminates with an optimal solution given by some basic feasible solution, say \( (u^*, w^*) \), with \( u^* \in \mathbb{R}^n \) and \( w^* \in \mathbb{R}^m \).

As in the proof of Theorem 26.7, for every feasible solution \( u \in \mathcal{P}(A, b) \) the vector \( (u, 0_m) \) is an optimal solution of (\( \hat{P} \)). Therefore, if \( w^* \neq 0 \), then \( \mathcal{P}(A, b) = \emptyset \), since otherwise for every feasible solution \( u \in \mathcal{P}(A, b) \) the vector \( (u, 0_m) \) would yield a value of the objective function \( -(x_{n+1} + \cdots + x_{n+m}) \) equal to 0, but \( (u^*, w^*) \) yields a strictly negative value since \( w^* \neq 0 \).

Otherwise, \( w^* = 0 \), and \( u^* \) is a feasible solution of (P). Since \( (u^*, 0_m) \) is a basic feasible solution of (\( \hat{P} \)) the columns corresponding to nonzero components of \( u^* \) are linearly independent. Some of the coordinates of \( u^* \) could be equal to 0, but since \( A \) has rank \( m \) we can add columns of \( A \) to obtain a basis \( K^* \) associated with \( u^* \), and \( u^* \) is indeed a basic feasible solution of (P).

Running the simplex algorithm on the linear program \( \hat{P} \) to obtain an initial feasible solution \( (u_0, K_0) \) of the linear program (P2) is called Phase I of the simplex algorithm. Running the simplex algorithm on the linear program (P2) with some initial feasible solution
10.3. HOW TO PERFORM A PIVOTING STEP EFFICIENTLY

\((u_0, K_0)\) is called Phase II of the simplex algorithm. If a feasible solution of the linear program \((P_2)\) is readily available then Phase I is skipped. Sometimes, at the end of Phase I, an optimal solution of \((P_2)\) is already obtained.

In summary, we proved the following fact worth recording.

**Proposition 10.1.** For any linear program \((P_2)\)

\[
\begin{align*}
\text{maximize} & \quad cx \\
\text{subject to} & \quad Ax = b \text{ and } x \geq 0,
\end{align*}
\]

in standard form, where \(A\) is an \(m \times n\) matrix of rank \(m\) and \(b \geq 0\), consider the linear program \(\hat{P}\) in standard form

\[
\begin{align*}
\text{maximize} & \quad -(x_{n+1} + \cdots + x_{n+m}) \\
\text{subject to} & \quad \hat{A}\hat{x} = b \text{ and } \hat{x} \geq 0.
\end{align*}
\]

The simplex algorithm with a pivot rule that prevents cycling started on the basic feasible solution \(\hat{x} = (0_n, b)\) of \(\hat{P}\) terminates with an optimal solution \((u^*, w^*)\).

1. If \(w^* \neq 0\), then \(\mathcal{P}(A, B) = \emptyset\), that is, the linear program \((P)\) has no feasible solution.
2. If \(w^* = 0\), then \(\mathcal{P}(A, B) \neq \emptyset\), and \(u^*\) is a basic feasible solution of \((P)\) associated with some basis \(K\).

Proposition 27.1 shows that determining whether the polyhedron \(\mathcal{P}(A, b)\) defined by a system of equations \(Ax = b\) and inequalities \(x \geq 0\) is nonempty is decidable. This decision procedure uses a fail-safe version of the simplex algorithm (that prevents cycling), and the proof that it always terminates and returns an answer is nontrivial.

10.3 How to Perform a Pivoting Step Efficiently

We now discuss briefly how to perform the computation of \((u^+, K^+)\) from a basic feasible solution \((u, K)\).

In order to avoid applying permutation matrices it is preferable to allow a basis \(K\) to be a sequence of indices, possibly out of order. Thus, for any \(m \times n\) matrix \(A\) (with \(m \leq n\)) and any sequence \(K = (k_1, k_2, \ldots, k_m)\) of \(m\) elements with \(k_i \in \{1, \ldots, n\}\), the matrix \(A_K\) denotes the \(m \times m\) matrix whose \(i\)th column is the \(k_i\)th column of \(A\), and similarly for any vector \(u \in \mathbb{R}^n\) (resp. any linear form \(c \in (\mathbb{R}^n)^*\)) the vector \(u_K \in \mathbb{R}^m\) (the linear form \(c_K \in (\mathbb{R}^m)^*\)) is the vector whose \(i\)th entry is the \(k_i\)th entry in \(u\) (resp. the linear whose \(i\)th entry is the \(k_i\)th entry in \(c\)).

For each nonbasic \(j \notin K\), we have

\[
A^j = \gamma^j_{k_1} A^{k_1} + \cdots + \gamma^j_{k_m} A^{k_m} = A_K \gamma^j_K,
\]
so the vector $\gamma^j_K$ is given by $\gamma^j_K = A^{-1}_K A^j$, that is, by solving the system

$$A_K \gamma^j_K = A^j. \quad (\ast_{\gamma})$$

To be very precise, since the vector $\gamma^j_K$ depends on $K$, its components should be denoted by $(\gamma^j_K)_k$, but as we said before, to simplify notation we write $\gamma^j_{K_k}$ instead of $(\gamma^j_K)_k$.

In order to decide which case applies ((A), (B1), (B2), (B3)), we need to compute the numbers $c_j - \sum_{k \in K} \gamma^j_k c_k$ for all $j \notin K$. For this, observe that

$$c_j - \sum_{k \in K} \gamma^j_k c_k = c_j - c_K \gamma^j_K = c_j - c_K A^{-1}_K A^j.$$

If we write $\beta_K = c_K A^{-1}_K$, then

$$c_j - \sum_{k \in K} \gamma^j_k c_k = c_j - \beta_K A^j.$$

and we see that $\beta^T_K \in \mathbb{R}^m$ is the solution of the system $\beta^T_K = (A^{-1}_K)^T c^T_K$, which means that $\beta^T_K$ is the solution of the system

$$A^T_K \beta^T_K = c^T_K. \quad (\ast_{\beta})$$

**Remark:** Observe that since $u$ is a basis feasible solution of $(P)$, we have $u_j = 0$ for all $j \notin K$, so $u$ is the solution of the equation $A_K u_K = b$. As a consequence, the value of the objective function for $u$ is $cu = c_K u_K = c_K A^{-1}_K b$. This fact will play a crucial role in Section 28.2 to show that when the simplex algorithm terminates with an optimal solution of the linear program $(P)$, then it also produces an optimal solution of the dual linear program $(D)$.

Assume that we have a basic feasible solution $u$, a basis $K$ for $u$, and that we also have the matrix $A_K$ as well its inverse $A^{-1}_K$ (perhaps implicitly) and also the inverse $(A^T_K)^{-1}$ of $A^T_K$ (perhaps implicitly). Here is a description of an iteration step of the simplex algorithm, following almost exactly Chvatal (Chvatal [29], Chapter 7, Box 7.1).

**An Iteration Step of the (Revised) Simplex Method**

**Step 1.** Compute the numbers $c_j - \sum_{k \in K} \gamma^j_k c_k = c_j - \beta_K A^j$ for all $j \notin K$, and for this, compute $\beta^T_K$ as the solution of the system

$$A^T_K \beta^T_K = c^T_K.$$

If $c_j - \beta_K A^j \leq 0$ for all $j \notin K$, stop and return the optimal solution $u$ (Case (A)).

**Step 2.** If Case (B) arises, use a pivot rule to determine which index $j^+ \notin K$ should enter the new basis $K^+$ (the condition $c_{j^+} - \beta_K A^{j^+} > 0$ should hold).

**Step 3.** Compute $\max_{k \in K} \gamma^{j^+}_k$. For this, solve the linear system

$$A_K \gamma^{j^+}_K = A^{j^+}.$$
10.3. HOW TO PERFORM A PIVOTING STEP EFFICIENTLY

Step 4. If $\max_{k \in K} \gamma^+_k \leq 0$, then stop and report that the linear program $(P)$ is unbounded (Case (B1)).

Step 5. If $\max_{k \in K} \gamma^+_k > 0$, use the ratios $u_k/\gamma^+_k$ for all $k \in K$ such that $\gamma^+_k > 0$ to compute $\theta^{j^+}$, and use a pivot rule to determine which index $k^- \in K$ such that $\theta^{j^+} = u_k^-/\gamma^+_{k^-}$ should leave $K$ (Case (B2)).

If $\max_{k \in K} \gamma^+_k = 0$, then use a pivot rule to determine which index $k$ for which $\gamma^-_{k} > 0$ should leave the basis $K$ (Case (B3)).

Step 6. Update $u$, $K$, and $A_K$, to $u^+$ and $K^+$, and $A_{K^+}$. During this step, given the basis $K$ specified by the sequence $K = (k_1, \ldots, k_\ell, \ldots, k_m)$, with $k^- = k_\ell$, then $K^+$ is the sequence obtained by replacing $k_\ell$ by the incoming index $j^+$, so $K^+ = (k_1, \ldots, j^+, \ldots, k_m)$ with $j^+$ in the $\ell$th slot.

The vector $u$ is easily updated. To compute $A_{K^+}$ from $A_K$ we take advantage that $A_K$ and $A_{K^+}$ only differ by a single column, namely the $\ell$th column $A_{j^+}$, which is given by the linear combination $A_{j^+} = A_K \gamma^+_{k^-}$.

To simplify notation, denote $\gamma^+_K$ by $\gamma$, and recall that $k^- = k_\ell$. If $K = (k_1, \ldots, k_m)$, then $A_K = [A^{k_1} \cdots A^{k_\ell} \cdots A^{k_m}]$, and since $A_{K^+}$ is the result of replacing the $\ell$th column $A^{k^-}$ of $A_K$ by the column $A^{j^+}$, we have

$$A_{K^+} = [A^{k_1} \cdots A^{j^+} \cdots A^{k_m}] = [A^{k_1} \cdots A_K \gamma \cdots A^{k_m}] = A_K E(\gamma),$$

where $E(\gamma)$ is the following invertible matrix obtained from the identity matrix $I_m$ by replacing its $\ell$th column by $\gamma$:

$$E(\gamma) = \begin{pmatrix}
1 & \gamma_1 & \cdots \\
& \ddots & \ddots & \ddots \\
& & 1 & \gamma_{\ell-1} & \gamma_\ell \\
& & & \gamma_{\ell+1} & 1 \\
& & & \ddots & \ddots \\
& & & & 1 & \gamma_m
\end{pmatrix}.$$

Since $\gamma_\ell = \gamma^+_k > 0$, the matrix $E(\gamma)$ is invertible, and it is easy to check that its inverse is given by

$$E(\gamma)^{-1} = \begin{pmatrix}
1 & -\gamma_\ell^{-1} \gamma_1 & \cdots \\
& \ddots & \ddots & \ddots \\
& & 1 & -\gamma_\ell^{-1} \gamma_{\ell-1} & \gamma_\ell^{-1} \\
& & & \gamma_{\ell+1}^{-1} & 1 \\
& & & \ddots & \ddots \\
& & & & -\gamma_\ell^{-1} \gamma_m & 1
\end{pmatrix},$$
which is very cheap to compute. We also have

$$A_{K^+}^{-1} = E(\gamma)^{-1} A_{K}^{-1}. \quad (\star)$$

Consequently, if $A_K$ and $A_{K}^{-1}$ are available, then $A_{K^+}$ and $A_{K^+}^{-1}$ can be computed cheaply in terms of $A_K$ and $A_{K}^{-1}$ and matrices of the form $E(\gamma)$. Then the systems $(\star_\gamma)$ to find the vectors $\gamma_{K^+}$ can be solved cheaply.

Since

$$A_{K^+}^\top = E(\gamma)^\top A_K^\top$$

and

$$(A_{K^+}^\top)^{-1} = (A_K^\top)^{-1} (E(\gamma)^\top)^{-1},$$

the matrices $A_{K^+}^\top$ and $(A_{K^+}^\top)^{-1}$ can also be computed cheaply from $A_K^\top$, $(A_K^\top)^{-1}$, and matrices of the form $E(\gamma)^\top$. Thus the systems $(\star_\beta)$ to find the linear forms $\beta_{K^+}$ can also be solved cheaply.

A matrix of the form $E(\gamma)$ is called an eta matrix; see Chvatal [29] (Chapter 7). We showed that the matrix $A_{K^+}$ obtained after $s$ steps of the simplex algorithm can be written as

$$A_{K^s} = A_{K^{s-1}} E_s$$

for some eta matrix $E_s$, so $A_{K^s}$ can be written as the product

$$A_{K^s} = E_1 E_2 \cdots E_s$$

of $s$ beta matrices. Such a factorization is called an eta factorization. The eta factorization can be used to either invert $A_{K^s}$ or to solve a system of the form $A_{K^s} \gamma = A_j^+$ iteratively. Which method is more efficient depends on the sparsity of the $E_i$.

In summary, there are cheap methods for finding the next basic feasible solution $(u^+, K^+)$ from $(u, K)$. We simply wanted to give the reader a flavor of these techniques. We refer the reader to texts on linear programming for detailed presentations of methods for implementing efficiently the simplex method. In particular, the revised simplex method is presented in Chvatal [29], Papadimitriou and Steiglitz [80], Bertsimas and Tsitsiklis [17], and Vanderbei [110].

### 10.4 The Simplex Algorithm Using Tableaux

We now describe a formalism for presenting the simplex algorithm, namely (full) tableaux. This is the traditional formalism used in all books, modulo minor variations. A particularly nice feature of the tableau formalism is that the update of a tableau can be performed using elementary row operations identical to the operations used during the reduction of a matrix to row reduced echelon form (rref). What differs is the criterion for the choice of the pivot.
10.4. THE SIMPLEX ALGORITHM USING TABLEAUX

Since the quantities $c_j - c_K \gamma^j_K$ play a crucial role in determining which column $A^j$ should come into the basis, the notation $\bar c_j$ is used to denote $c_j - c_K \gamma^j_K$, which is called the reduced cost of the variable $x_j$. The reduced costs actually depend on $K$ so to be very precise we should denote them by $(\bar c_K)_{j}$, but to simplify notation we write $\bar c_j$ instead of $(\bar c_K)_{j}$. We will see shortly how $(\bar c_K)_{i}$ is computed in terms of the $(\bar c_K)_{i}$.

Observe that the data needed to execute the next step of the simplex algorithm are
(1) The current basic solution $u_K$ and its basis $K = (k_1, \ldots, k_m)$.
(2) The reduced costs $\bar c_j = c_j - c_K A^{-1}_K A^j = c_j - c_K \gamma^j_K$, for all $j \notin K$.
(3) The vectors $\gamma^j_K = (\gamma^j_{K_i})_{i=1}^m$ for all $j \notin K$, that allow us to express each $A^j$ as $A^j K \gamma^j_K$.

All this information can be packed into a $(m+1) \times (n+1)$ matrix called a (full) tableau organized as follows:

| $c_K u_K$ | $\bar c_1$ | $\cdots$ | $\bar c_j$ | $\cdots$ | $\bar c_n$ |
|-----------|------------|----------|------------|----------|
| $u_{k_1}$ | $\gamma^1_1$ | $\cdots$ | $\gamma^j_1$ | $\cdots$ | $\gamma^1_n$ |
| $\vdots$  | $\vdots$    | $\vdots$ | $\vdots$   | $\vdots$ |
| $u_{k_m}$ | $\gamma^1_m$ | $\cdots$ | $\gamma^j_m$ | $\cdots$ | $\gamma^m_n$ |

It is convenient to think as the first row as row 0, and of the first column as column 0. Row 0 contains the current value of the objective function and the reduced costs, column 0 except for its top entry contains the components of the current basic solution $u_K$, and the remaining columns except for their top entry contain the vectors $\gamma^j_K$. Observe that the $\gamma^j_K$ corresponding to indices $j$ in $K$ constitute a permutation of the identity matrix $I_m$. The entry $\gamma^j_{K_k}$ is called the pivot element. A tableau together with the new basis $K^+ = (K - \{k^-\}) \cup \{j^+\}$ contains all the data needed to compute the new $u_{K^+}$, the new $\gamma^j_{K^+}$, and the new reduced costs $(\bar c_{K^+})_{j}$.

If we define the $m \times n$ matrix $\Gamma$ as the matrix $\Gamma = [\gamma^1_K \cdots \gamma^n_K]$ whose $j$th column is $\gamma^j_K$, and $\bar c$ as the row vector $\bar c = (\bar c_1 \cdots \bar c_n)$, then the above tableau is denoted concisely by

<table>
<thead>
<tr>
<th>$c_K u_K$</th>
<th>$\bar c$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$u_K$</td>
<td>$\Gamma$</td>
</tr>
</tbody>
</table>

We now show that the update of a tableau can be performed using elementary row operations identical to the operations used during the reduction of a matrix to row reduced echelon form (rref).

If $K = (k_1, \ldots, k_m)$, $j^+$ is the index of the incoming basis vector, $k^- = k_\ell$ is the index of the column leaving the basis, and if $K^+ = (k_1, \ldots, k_{\ell-1}, j^+, k_{\ell+1}, \ldots, k_m)$, since $A_{K^+} = A_K E(\gamma^j_{K^+})$, the new columns $\gamma^j_{K^+}$ are computed in terms of the old columns $\gamma^j_K$ using the equations

$$\gamma^j_{K^+} = A_{K^+}^{-1} A^j = E(\gamma^j_{K^+})^{-1} A_K^{-1} A^j = E(\gamma^j_K)^{-1} \gamma^j_K.$$
Consequently the matrix $\Gamma^+$ is given in terms of $\Gamma$ by

$$
\Gamma^+ = E(\gamma^+_K)^{-1}\Gamma.
$$

But the matrix $E(\gamma^+_K)^{-1}$ is of the form

$$
E(\gamma)^{-1} = \begin{pmatrix}
1 & -\gamma^+_1 & \cdots & -\gamma^+_1 \\
& \ddots & & \vdots \\
& & 1 & -\gamma^+_l \\
& & & \ddots & \gamma^+_1 \\
& & & & \cdots \\
& & & & 1
\end{pmatrix},
$$

with the column involving the $\gamma$s in the $\ell$th column, and this matrix is the product of the following elementary row operations:

1. Multiply row $\ell$ by $1/\gamma^+_k$ (the inverse of the pivot) to make the entry on row $\ell$ and column $j^+$ equal to 1.

2. Subtract $\gamma^+_k \times$ (the normalized) row $\ell$ from row $i$, for $i = 1, \ldots, \ell - 1, \ell + 1, \ldots, m$.

These are exactly the elementary row operations that reduce the $\ell$th column $\gamma^+_K$ of $\Gamma$ to the $\ell$th column of the identity matrix $I_m$. Thus, this step is identical to the sequence of steps that the procedure to convert a matrix to row reduced echelon from executes on the $\ell$th column of the matrix. The only difference is the criterion for the choice of the pivot.

Since the new basic solution $u_{K^+}$ is given by $u_{K^+} = A_{K^+}^{-1}b$, we have

$$
u_{K^+} = E(\gamma^+_K)^{-1}A_{K^+}^{-1}b = E(\gamma^+_K)^{-1}u_K.
$$

This means that $u_+$ is obtained from $u_K$ by applying exactly the same elementary row operations that were applied to $\Gamma$. Consequently, just as in the procedure for reducing a matrix to rref, we can apply elementary row operations to the matrix $[u_k \Gamma]$, which consists of rows $1, \ldots, m$ of the tableau.

Once the new matrix $\Gamma^+$ is obtained, the new reduced costs are given by the following proposition.

**Proposition 10.2.** Given any linear program $(P2)$ is standard form

$$
\text{maximize } cx \\
\text{subject to } Ax = b \text{ and } x \geq 0,
$$
where $A$ is an $m \times n$ matrix of rank $m$, if $(u, K)$ is a basic (not feasible) solution of $(P2)$ and if $K^+ = (K - \{k^\circ\}) \cup \{j^+\}$, with $K = (k_1, \ldots, k_m)$ and $k^\circ = k_\ell$, then for $i = 1, \ldots, n$ we have

$$c_i - c_{K^+}, \gamma_{K^+}^i = c_i - c_K, \gamma_K^i - \frac{\gamma_{K^+}^i}{\gamma_{K^\circ}^i} (c_{j^+} - c_K, \gamma_{K^\circ}^j).$$

Using the reduced cost notation, the above equation is

$$(\bar{c}_{K^+})_i = (\bar{c}_K)_i - \frac{\gamma_{K^\circ}^i}{\gamma_{K^\circ}^j} (\bar{c}_K)_{j^+}.$$ 

Proof. Without any loss of generality and to simplify notation assume that $K = (1, \ldots, m)$ and write $j$ for $j^+$ and $\ell$ for $k_m$. Since $\gamma_K^i = A_K^{-1} A^i$, $\gamma_{K^+}^i = A_{K^+}^{-1} A^i$, and $A_{K^+} = A_K E(\gamma_K^i)$, we have

$$c_i - c_{K^+}, \gamma_{K^+}^i = c_i - c_K, A_K^{-1} A^i = c_i - c_{K^+}, E(\gamma_K^i)^{-1} A_K^{-1} A^i = c_i - c_{K^+}, E(\gamma_K^i)^{-1} \gamma_K^i,$$

where

$$E(\gamma_K^i)^{-1} = \begin{pmatrix} 1 & -\gamma_1^i & \cdots & -\gamma_{\ell-1}^i & 1 \\ -\gamma_1^i & 1 & \cdots & -\gamma_{\ell-1}^i & -\gamma_\ell^i \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ -\gamma_{\ell-1}^i & \cdots & 1 & -\gamma_\ell^i \\ -\gamma_\ell^i & \cdots & -\gamma_\ell^i & 1 \end{pmatrix},$$

where the $\ell$th column contains the $\gamma$s. Since $c_{K^+} = (c_1, \ldots, c_{\ell-1}, c_j, c_{\ell+1}, \ldots, c_m)$, we have

$$c_{K^+}, E(\gamma_K^i)^{-1} = \left( c_1, \ldots, c_{\ell-1}, \frac{c_j}{\gamma_\ell^i} - \sum_{k=1, k\neq \ell}^{m} c_k \frac{\gamma_k^j}{\gamma_\ell^i}, c_{\ell+1}, \ldots, c_m \right).$$
and

\[
c_{K^+}E(\gamma_k^j)^{-1}\gamma_K^i = \left( c_1 \ldots c_{\ell-1} \frac{c_j}{\gamma_{\ell}^j} - \sum_{k=1,k \neq \ell}^{m} c_k \frac{\gamma_k^j}{\gamma_{\ell}^j} c_{\ell+1} \ldots c_m \right) \begin{pmatrix} \gamma_1^i \\ \vdots \\ \gamma_{\ell}^i \\ \gamma_{\ell+1}^i \\ \vdots \\ \gamma_m^i \end{pmatrix}
\]

\[
= \sum_{k=1,k \neq \ell}^{m} c_k \gamma_k^j + \frac{\gamma_{\ell}^i}{\gamma_{\ell}^j} \left( c_j - \sum_{k=1,k \neq \ell}^{m} c_k \gamma_k^j \right)
\]

\[
= \sum_{k=1,k \neq \ell}^{m} c_k \gamma_k^j + \frac{\gamma_{\ell}^i}{\gamma_{\ell}^j} \left( c_j + c_{\ell} \gamma_{\ell}^j - \sum_{k=1}^{m} c_k \gamma_k^j \right)
\]

\[
= \sum_{k=1}^{m} c_k \gamma_k^j + \frac{\gamma_{\ell}^i}{\gamma_{\ell}^j} \left( c_j - \sum_{k=1}^{m} c_k \gamma_k^j \right)
\]

\[
= c_K \gamma_K^i + \frac{\gamma_{\ell}^i}{\gamma_{\ell}^j} (c_j - c_K \gamma_K^j),
\]

and thus

\[
c_i - c_{K^+} \gamma_{K^+}^i = c_i - c_{K^+} E(\gamma_K^j)^{-1}\gamma_K^i = c_i - c_K \gamma_K^i - \frac{\gamma_{\ell}^i}{\gamma_{\ell}^j} (c_j - c_K \gamma_K^j),
\]

as claimed. \(\Box\)

Since \((\gamma_{k-1}^1, \ldots, \gamma_{k-}^n)\) is the \(\ell\)-th row of \(\Gamma\), we see that Proposition 27.2 shows that

\[
\bar{c}_{K^+} = \bar{c}_K - \frac{(\bar{c}_{K^+})_{j^+}}{\gamma_{k^+}^j} \Gamma_\ell, \tag{\dag}
\]

where \(\Gamma_\ell\) denotes the \(\ell\)-th row of \(\Gamma\) and \(\gamma_{k^+}^j\) is the pivot. This means that \(\bar{c}_{K^+}\) is obtained by the elementary row operations which consist first normalizing the \(\ell\)-th row by dividing it by the pivot \(\gamma_{k^+}^j\), and then subtracting \((\bar{c}_K)_{j^+} \times \gamma_{k^+}^j\) from \(\bar{c}_K\). These are exactly the row operations that make the reduced cost \((\bar{c}_K)_{j^+}\) zero.

**Remark:** It easy easy to show that we also have

\[
\bar{c}_{K^+} = c - c_{K^+}\Gamma^+.
\]
We saw in section 27.2 that the change in the objective function after a pivoting step during which column $j^+$ comes in and column $k^-$ leaves is given by
\[
\theta^{j^+} \left( c_{j^+} - \sum_{k \in K} \gamma_k^{j^+} c_k \right) = \theta^{j^+} (\bar{c}_K)_{j^+},
\]
where
\[
\theta^{j^+} = \frac{u_{k^-}}{\gamma_k^{j^+}}.
\]
If we denote the value of the objective function $c_K u_K$ by $z_K$, then we see that
\[
z_{K^+} = z_K + \frac{(\bar{c}_K)_{j^+}}{\gamma_k^{j^+}} u_{k^-}.
\]
This means that the new value $z_{K^+}$ of the objective function is obtained by first normalizing the $\ell$th row by dividing it by the pivot $\gamma_k^{j^+}$, and then adding $(\bar{c}_K)_{j^+} \times$ the zeroth entry of the normalized $\ell$th line by $(\bar{c}_K)_{j^+}$ to the zeroth entry of line 0.

In updating the reduced costs, we subtract rather than add $(\bar{c}_K)_{j^+} \times$ the normalized row $\ell$ from row 0. This suggests storing $-z_K$ as the zeroth entry on line 0 rather than $z_K$, because then all the entries row 0 are updated by the same elementary row operations. Therefore, from now on, we use tableau of the form

| $-c_K u_K$ | $\bar{c}_1$ | $\cdots$ | $\bar{c}_j$ | $\cdots$ | $\bar{c}_n$ |
|------------|-------------|-----------|-------------|-----------|
| $u_{k1}$ | $\gamma_1^1$ | $\cdots$ | $\gamma_1^j$ | $\cdots$ | $\gamma_1^n$ |
| $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ |
| $u_{km}$ | $\gamma_m^1$ | $\cdots$ | $\gamma_m^j$ | $\cdots$ | $\gamma_m^n$ |

The simplex algorithm first chooses the incoming column $j^+$ by picking some column for which $\bar{c}_j > 0$, and then chooses the outgoing column $k^-$ by considering the ratios $u_k/\gamma_k^{j^+}$ for which $\gamma_k^{j^+} > 0$ (along column $j^+$), and picking $k^-$ to achieve the minimum of these ratios.

Here is an illustration of the simplex algorithm using elementary row operations on an example from Papadimitriou and Steiglitz [80] (Section 2.9).

**Example 10.4.** Consider the linear program

maximize $-2x_2 - x_4 - 5x_7$

subject to

\[
\begin{align*}
x_1 + x_2 + x_3 + x_4 &= 4 \\
x_1 + x_5 &= 2 \\
x_3 + x_6 &= 3 \\
3x_2 + x_3 + x_7 &= 6 \\
x_1, x_2, x_3, x_4, x_5, x_6, x_7 &\geq 0.
\end{align*}
\]
We have the basic feasible solution \( u = (0, 0, 4, 2, 3, 6) \), with \( K = (4, 5, 6, 7) \). Since \( c_K = (-1, 0, 0, -5) \) and \( c = (0, -2, 0, -1, 0, 0, -5) \) the first tableau is

\[
\begin{array}{cccccccc}
34 & 1 & 14 & 6 & 0 & 0 & 0 & 0 \\
u_4 = 4 & 1 & 1 & 1 & 1 & 0 & 0 & 0 \\
u_5 = 2 & \textbf{1} & 0 & 0 & 0 & 1 & 0 & 0 \\
u_6 = 3 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\
u_7 = 6 & 0 & 3 & 1 & 0 & 0 & 0 & 1 \\
\end{array}
\]

Row 0 is obtained by subtracting \(-1\times\) (row 1) and \(-5\times\) (row 4) from \( c = (0, -2, 0, -1, 0, 0, -5) \). Let us pick column \( j^+ = 1 \) as the incoming column. We have the ratios (for positive entries on column 1)

\[
4/1, 2/1,
\]

and since the minimum is 2, we pick the outgoing column to be column \( k^- = 5 \). The pivot 1 is indicated in red. The new basis is \( K = (4, 1, 6, 7) \). Next we apply row operations to reduce column 1 to the second vector of the identity matrix \( I_4 \). For this, we subtract row 2 from row 1. We get the tableau

\[
\begin{array}{cccccccc}
32 & 0 & 14 & 6 & 0 & -1 & 0 & 0 \\
u_4 = 2 & 0 & 1 & 1 & 1 & -1 & 0 & 0 \\
u_1 = 2 & \textbf{1} & 0 & 0 & 0 & 1 & 0 & 0 \\
u_6 = 3 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\
u_7 = 6 & 0 & 3 & 1 & 0 & 0 & 0 & 1 \\
\end{array}
\]

To compute the new reduced costs, we want to set \( \pi_1 \) to 0 so we subtract row 2 from row 0, and we get the tableau

\[
\begin{array}{cccccccc}
32 & 0 & 14 & 6 & 0 & -1 & 0 & 0 \\
u_4 = 2 & 0 & 1 & \textbf{1} & 1 & -1 & 0 & 0 \\
u_1 = 2 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\
u_6 = 3 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\
u_7 = 6 & 0 & 3 & 1 & 0 & 0 & 0 & 1 \\
\end{array}
\]

Next, pick column \( j^+ = 3 \) as the incoming column. We have the ratios (for positive entries on column 3)

\[
2/1, 3/1, 6/1,
\]

and since the minimum is 2, we pick the outgoing column to be column \( k^- = 4 \). The pivot 1 is indicated in red and the new basis is \( K = (3, 1, 6, 7) \). Next we apply row operations to reduce column 3 to the first vector of the identity matrix \( I_4 \). For this, we subtract row 1 from row 3 and from row 4, to obtain the tableau:
To compute the new reduced costs, we want to set $c_3$ to 0 so we subtract $6 \times$ row 1 from row 0, and we get the tableau

<table>
<thead>
<tr>
<th>32</th>
<th>0</th>
<th>14</th>
<th>6</th>
<th>0</th>
<th>-1</th>
<th>0</th>
<th>0</th>
</tr>
</thead>
<tbody>
<tr>
<td>$u_3 = 2$</td>
<td>0</td>
<td>1</td>
<td>(1)</td>
<td>1</td>
<td>-1</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$u_1 = 2$</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$u_6 = 1$</td>
<td>0</td>
<td>-1</td>
<td>0</td>
<td>-1</td>
<td>1</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>$u_7 = 4$</td>
<td>0</td>
<td>2</td>
<td>0</td>
<td>-1</td>
<td>1</td>
<td>0</td>
<td>1</td>
</tr>
</tbody>
</table>

Next we pick $j^+ = 2$ as the incoming column. We have the ratios (for positive entries on column 2)

$$\frac{2}{1}, \frac{4}{2},$$

and since the minimum is 2, we pick the outgoing column to be column $k^- = 3$. The pivot 1 is indicated in red and the new basis is $K = (2, 1, 6, 7)$. Next we apply row operations to reduce column 2 to the first vector of the identity matrix $I_4$. For this, we add row 1 to row 3 and subtract $2 \times$ row 1 from row 4 to obtain the tableau:

<table>
<thead>
<tr>
<th>20</th>
<th>0</th>
<th>8</th>
<th>0</th>
<th>-6</th>
<th>5</th>
<th>0</th>
<th>0</th>
</tr>
</thead>
<tbody>
<tr>
<td>$u_2 = 2$</td>
<td>0</td>
<td>(1)</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$u_1 = 2$</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$u_6 = 3$</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>$u_7 = 0$</td>
<td>0</td>
<td>0</td>
<td>-2</td>
<td>-3</td>
<td>3</td>
<td>0</td>
<td>1</td>
</tr>
</tbody>
</table>

To compute the new reduced costs, we want to set $c_2$ to 0 so we subtract $8 \times$ row 1 from row 0 and we get the tableau

<table>
<thead>
<tr>
<th>4</th>
<th>0</th>
<th>0</th>
<th>-8</th>
<th>-14</th>
<th>13</th>
<th>0</th>
<th>0</th>
</tr>
</thead>
<tbody>
<tr>
<td>$u_2 = 2$</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$u_1 = 2$</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$u_6 = 3$</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>$u_7 = 0$</td>
<td>0</td>
<td>0</td>
<td>-2</td>
<td>-3</td>
<td>3</td>
<td>0</td>
<td>1</td>
</tr>
</tbody>
</table>

The only possible incoming column corresponds to $j^+ = 5$. We have the ratios (for positive entries on column 5)

$$\frac{2}{1}, \frac{0}{3},$$
and since the minimum is 0, we pick the outgoing column to be column $k^− = 7$. The pivot 3 is indicated in red and the new basis is $K = (2, 1, 6, 5)$. Since the minimum is 0, the basis $K = (2, 1, 6, 5)$ is degenerate (indeed, the component corresponding to the index 5 is 0).

Next we apply row operations to reduce column 5 to the fourth vector of the identity matrix $I_4$. For this, we multiply row 4 by $1/3$, and then add the normalized row 4 to row 1 and subtract the normalized row 4 from row 2, and to obtain the tableau:

$$
\begin{array}{ccccccc}
4 & 0 & 0 & -8 & -14 & 13 & 0 & 0 \\
\mu_2 = 2 & 0 & 1 & 1/3 & 0 & 0 & 0 & 1/3 \\
\mu_1 = 2 & 1 & 0 & 2/3 & 1 & 0 & 0 & -1/3 \\
\mu_6 = 3 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\
\mu_5 = 0 & 0 & 0 & -2/3 & -1 & 1 & 0 & 1/3 \\
\end{array}
$$

To compute the new reduced costs, we want to set $\bar{c}_5$ to 0 so we subtract $13 \times$ row 4 from row 0 and we get the tableau

$$
\begin{array}{ccccccc}
4 & 0 & 0 & 2/3 & -1 & 0 & 0 & -13/3 \\
\mu_2 = 2 & 0 & 1 & 1/3 & 0 & 0 & 0 & 1/3 \\
\mu_1 = 2 & 1 & 0 & (2/3) & 1 & 0 & 0 & -1/3 \\
\mu_6 = 3 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\
\mu_5 = 0 & 0 & 0 & -2/3 & -1 & 1 & 0 & 1/3 \\
\end{array}
$$

The only possible incoming column corresponds to $j^+ = 3$. We have the ratios (for positive entries on column 3)

$$
2/(1/3) = 6, \quad 2/(2/3) = 3, \quad 3/1 = 3,
$$

and since the minimum is 3, we pick the outgoing column to be column $k^− = 1$. The pivot 2/3 is indicated in red and the new basis is $K = (2, 3, 6, 5)$. Next we apply row operations to reduce column 3 to the second vector of the identity matrix $I_4$. For this, we multiply row 2 by 2/3, subtract $(1/3) \times$ (normalized row 2) from row 1, and subtract normalized row 2 from row 3, add row $(2/3) \times$ (normalized row 2) to row 4, to obtain the tableau:

$$
\begin{array}{ccccccc}
4 & 0 & 0 & 2/3 & -1 & 0 & 0 & -13/3 \\
\mu_2 = 1 & -1/2 & 1 & 0 & -1/2 & 0 & 0 & 1/2 \\
\mu_3 = 3 & 3/2 & 0 & 1 & 3/2 & 0 & 0 & -1/2 \\
\mu_6 = 0 & -3/2 & 0 & 0 & -3/2 & 0 & 1 & 1/2 \\
\mu_5 = 2 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\
\end{array}
$$

To compute the new reduced costs, we want to set $\bar{c}_3$ to 0 so we subtract $(2/3) \times$ row 2 from row 0 and we get the tableau
Since all the reduced cost are \( \leq 0 \), we have reached an optimal solution, namely \((0, 1, 3, 0, 2, 0, 0, 0)\), with optimal value \(-2\).

The progression of the simplex algorithm from one basic feasible solution to another corresponds to the visit of vertices of the polyhedron \( \mathcal{P} \) associated with the constraints of the linear program illustrated in Figure 27.4.

As a final comment, if it is necessary to run Phase I of the simplex algorithm, in the event that the simplex algorithm terminates with an optimal solution \((u^*, 0_m)\) and a basis \(K^*\) such that some \(u_i = 0\), then the basis \(K^*\) contains indices of basic columns \(A_j^t\) corresponding to slack variables that need to be driven out of the basis. This is easy to achieve by performing a pivoting step involving some other column \(j^+\) corresponding to one of the original variables (not a slack variable) for which \((\gamma_{K^*})_i^+ \neq 0\). In such a step, it doesn’t matter whether \((\gamma_{K^*})_i^+ < 0\) or \((\tau_{K^*})_j^+ \leq 0\). If the original matrix \(A\) has no redundant equations, such a step
is always possible. Otherwise, \((\gamma_{K_i^*})_i^2 = 0\) for all non-slack variables, so we detected that the
ith equation is redundant and we can delete it.

Other presentations of the tableau method can be found in Bertsimas and Tsitsiklis [17] and Papadimitriou and Steiglitz [80].

10.5 Computational Efficiency of the Simplex Method

Let us conclude with a few comments about the efficiency of the simplex algorithm. In
practice, it was observed by Dantzig that for linear programs with \(m < 50\) and \(m + n < 200\),
the simplex algorithms typically requires less than \(3m/2\) iterations, but at most \(3m\) iterations.
This fact agrees with more recent empirical experiments with much larger programs that
show that the number iterations is bounded by \(3m\). Thus, it was somewhat of a shock in
1972 when Klee and Minty found a linear program with \(n\) variables and \(n\) equations for
which the simplex algorithm with Dantzig’s pivot rule requires requires \(2^n - 1\) iterations.
This program (taken from Chvatal [29], page 47) is reproduced below:

\[
\begin{align*}
\text{maximize} & \quad \sum_{j=1}^{n} 10^{n-j} x_j \\
\text{subject to} & \quad \left( 2 \sum_{j=1}^{i-1} 10^{i-j} x_j \right) + x_i \leq 100^{i-1} \\
x_j & \geq 0,
\end{align*}
\]

for \(i = 1, \ldots, n\) and \(j = 1, \ldots, n\).

If \(p = \max(m, n)\), then , in terms of worse case behavior, for all currently known pivot
rules, the simplex algorithm has exponential complexity in \(p\). However, as we said earlier, in
practice, nasty examples such as the Klee–Minty example seem to be rare, and the number
of iterations appears to be linear in \(m\).

Whether or not a pivot rule (a clairvoyant rule) for which the simplex algorithms runs
in polynomial time in terms of \(m\) is still an open problem.

The Hirsch conjecture claims that there is some pivot rule such that the simplex algorithm
finds an optimal solution in \(O(p)\) steps. The best bound known so far due to Kalai and
Kleitman is \(m^{1+\ln n} = (2n)^{\ln m}\). For more on this topic, see Matousek and Gardner [73]
(Section 5.9) and Bertsimas and Tsitsiklis [17] (Section 3.7).

Researchers have investigated the problem of finding upper bounds on the expected
number of pivoting steps if a randomized pivot rule is used. Bounds better than \(2^m\) (but of
course, not polynomial) have been found.
Understanding the complexity of linear programming, in particular of the simplex algorithm, is still ongoing. The interested reader is referred to Matousek and Gardner [73] (Chapter 5, Section 5.9) for some pointers.

In the next section we consider important theoretical criteria for determining whether a set of constraints $Ax \leq b$ and $x \geq 0$ has a solution or not.
Chapter 11
Linear Programming and Duality

11.1 Variants of the Farkas Lemma

If $A$ is an $m \times n$ matrix and if $b \in \mathbb{R}^m$ is a vector, it is known from linear algebra that the linear system $Ax = b$ has no solution iff there is some linear form $y \in (\mathbb{R}^m)^*$ such that $yA = 0$ and $yb \neq 0$. This means that the linear form $y$ vanishes on the columns $A^1, \ldots, A^n$ of $A$ but does not vanish on $b$. Since the linear form $y$ defines the linear hyperplane $H$ of equation $yz = 0$ (with $z \in \mathbb{R}^m$), geometrically the equation $Ax = b$ has no solution iff there is a linear hyperplane $H$ containing $A^1, \ldots, A^n$ and not containing $b$. This is a kind of separation theorem that says that the vectors $A^1, \ldots, A^n$ and $b$ can be separated by some linear hyperplane $H$.

What we would like to do is to generalize this kind of criterion, first to a system $Ax = b$ subject to the constraints $x \geq 0$, and next to sets of inequality constraints $Ax \leq b$ and $x \geq 0$. There are indeed such criteria going under the name of Farkas lemma.

The key is a separation result involving polyhedral cones known as the Farkas–Minkowski proposition. We have the following fundamental separation lemma.

Proposition 11.1. Let $C \subseteq \mathbb{R}^n$ be a closed nonempty cone. For any point $a \in \mathbb{R}^n$, if $a \notin C$, then there is a linear hyperplane $H$ (through $0$) such that

1. $C$ lies in one of the two half-spaces determined by $H$.
2. $a \notin H$
3. $a$ lies in the other half-space determined by $H$.

We say that $H$ strictly separates $C$ and $a$.

Proposition 28.1 is an easy consequence of another separation theorem that asserts that given any two nonempty closed convex sets $A$ and $B$ with $A$ compact, there is a hyperplane $H$ strictly separating $A$ and $B$ (which means that $A \cap H = \emptyset$, $B \cap H = \emptyset$, that $A$ lies in one
of the two half-spaces determined by $H$, and $B$ lies in the other half-space determined by $H$); see Gallier [44] (Chapter 7, Corollary 7.4 and Proposition 7.3). This proof is nontrivial and involves a geometric version of the Hahn–Banach theorem.

The Farkas–Minkowski proposition is Proposition 28.1 applied to a polyhedral cone

$$ C = \{ \lambda_1 a_1 + \cdots + \lambda_n a_n \mid \lambda_i \geq 0, \ i = 1, \ldots, n \} $$

where $\{a_1, \ldots, a_n\}$ is a finite number of vectors $a_i \in \mathbb{R}^n$. By Proposition 25.2, any polyhedral cone is closed, so Proposition 28.1 applies and we obtain the following separation lemma.

**Proposition 11.2.** (Farkas–Minkowski) Let $C \subseteq \mathbb{R}^n$ be a nonempty polyhedral cone $C = \text{cone}(\{a_1, \ldots, a_n\})$. For any point $b \in \mathbb{R}^n$, if $b \notin C$, then there is a linear hyperplane $H$ (through 0) such that

1. $C$ lies in one of the two half-spaces determined by $H$.
2. $a \notin H$
3. $a$ lies in the other half-space determined by $H$.

Equivalently, there is a nonzero linear form $y \in (\mathbb{R}^n)^*$ such that

1. $y a_i \geq 0$ for $i = 1, \ldots, n$.
2. $y b < 0$.

A direct proof of the Farkas–Minkowski proposition not involving Proposition 28.1 is given at the end of this section.

**Remark:** There is a generalization of the Farkas–Minkowski proposition applying to infinite dimensional real Hilbert spaces; see Theorem 29.11 (or Ciarlet [30], Chapter 9).

Proposition 28.2 implies our first version of Farkas’ lemma.

**Proposition 11.3.** (Farkas Lemma, Version I) Let $A$ be an $m \times n$ matrix and let $b \in \mathbb{R}^m$ be any vector. The linear system $Ax = b$ has no solution $x \geq 0$ iff there is some nonzero linear form $y \in (\mathbb{R}^m)^*$ such that $y A \geq 0^T$ and $y b < 0$.

**Proof.** First, assume that there is some nonzero linear form $y \in (\mathbb{R}^m)^*$ such that $y A \geq 0$ and $y b < 0$. If $x \geq 0$ is a solution of $Ax = b$, then we get

$$ y A x = y b, $$

but if $y A \geq 0$ and $x \geq 0$, then $y Ax \geq 0$, and yet by hypothesis $y b < 0$, a contradiction.

Next assume that $Ax = b$ has no solution $x \geq 0$. This means that $b$ does not belong to the polyhedral cone $C = \text{cone}(\{A^1, \ldots, A^n\})$ spanned by the columns of $A$. By Proposition 28.2, there is a nonzero linear form $y \in (\mathbb{R}^m)^*$ such that
1. $yA^j \geq 0$ for $j = 1, \ldots, n$.

2. $yb < 0$,

which says that $yA \geq 0^n$ and $yb < 0$. \hfill \Box

Next consider the solvability of a system of inequalities of the form $Ax \leq b$ and $x \geq 0$.

**Proposition 11.4.** (Farkas Lemma, Version II) Let $A$ be an $m \times n$ matrix and let $b \in \mathbb{R}^n$ be any vector. The system of inequalities $Ax \leq b$ has no solution $x \geq 0$ iff there is some nonzero linear form $y \in (\mathbb{R}^m)^*$ such that $y \geq 0^m$, $yA \geq 0^n$, and $yb < 0$.

**Proof.** We use the trick of linear programming which consists of adding “slack variables” $z_i$ to convert inequalities $a_i x \leq b_i$ into equations $a_i x + z_i = b_i$ with $z_i \geq 0$ already discussed just before Definition 25.5. If we let $z = (z_1, \ldots, z_m)$, it is obvious that the system $Ax \leq b$ has a solution $x \geq 0$ iff the equation

$$(A \ I_m) \begin{pmatrix} x \\ z \end{pmatrix} = b$$

has a solution $\begin{pmatrix} x \\ z \end{pmatrix}$ with $x \geq 0$ and $z \geq 0$. Now by Farkas I, the above system has no solution with with $x \geq 0$ and $z \geq 0$ iff there is some nonzero linear form $y \in (\mathbb{R}^m)^*$ such that

$$y (A \ I_m) \geq 0^m_{n+m}$$

and $yb < 0$, that is, $yA \geq 0^n$, $y \geq 0^m$, and $yb < 0$. \hfill \Box

In the next section we use Farkas II to prove the duality theorem in linear programming. Observe that by taking the negation of the equivalence in Farkas II we obtain a criterion of solvability, namely:

The system of inequalities $Ax \leq b$ has a solution $x \geq 0$ iff for every nonzero linear form $y \in (\mathbb{R}^m)^*$ such that $y \geq 0^m$, if $yA \geq 0^n$, then $yb \geq 0$.

We now prove the Farkas–Minkowski proposition without using Proposition 28.1. This approach uses a basic property of the distance function from a point to a closed set.

Let $X \subseteq \mathbb{R}^n$ be any nonempty set and let $a \in \mathbb{R}^n$ be any point. The distance $d(a, X)$ from $a$ to $X$ is defined as

$$d(a, X) = \inf_{x \in X} \|a - x\|.$$

Here, $\| \|$ denotes the Euclidean norm.

**Proposition 11.5.** Let $X \subseteq \mathbb{R}^n$ be any nonempty set and let $a \in \mathbb{R}^n$ be any point. If $X$ is closed, then there is some $z \in X$ such that $\|a - z\| = d(a, X)$. 
Proof. Since $X$ is nonempty, pick any $x_0 \in X$, and let $r = \|a - x_0\|$. If $B_r(a)$ is the closed ball $B_r(a) = \{x \in \mathbb{R}^n \mid \|x - a\| \leq r\}$, then clearly
\[
d(a, X) = \inf_{x \in X} \|a - x\| = \inf_{x \in X \cap B_r(a)} \|a - x\|.
\]
Since $B_r(a)$ is compact and $X$ is closed, $K = X \cap B_r(a)$ is also compact. But the function $x \mapsto \|a - x\|$ defined on the compact set $K$ is continuous, and the image of a compact set by a continuous function is compact, so by Heine–Borel it has a minimum that is achieved by some $z \in K \subseteq X$. \qed

Remark: If $U$ is a nonempty, closed and convex subset of a Hilbert space $V$, a standard result of Hilbert space theory (the projection theorem) asserts that for any $v \in V$ there is a unique $p \in U$ such that
\[
\|v - p\| = \inf_{u \in U} \|v - u\| = d(v, U),
\]
and
\[
\langle p - v, u - p \rangle \geq 0 \quad \text{for all } u \in U.
\]
Here $\|w\| = \sqrt{\langle w, w \rangle}$, where $\langle -, - \rangle$ is the inner product of the Hilbert space $V$.

We can now give a proof of the Farkas–Minkowski proposition (Proposition 28.2).

Proof of the Farkas–Minkowski proposition. Let $C = \text{cone} \{a_1, \ldots, a_m\}$ be a polyhedral cone (nonempty) and assume that $b \notin C$. By Proposition 25.2, the polyhedral cone is closed, and by Proposition 28.5 there is some $z \in C$ such that $d(b, C) = \|b - z\|$, that is, $z$ is a point of $C$ closest to $b$. Since $b \notin C$ and $z \in C$ we have $u = z - b \neq 0$, and we claim that the linear hyperplane $H$ orthogonal to $u$ does the job, as illustrated in Figure 28.1.

First let us show that
\[
\langle u, z \rangle = \langle z - b, z \rangle = 0. \quad (\star_1)
\]
This is trivial if $z = 0$, so assume $z \neq 0$. If $\langle u, z \rangle \neq 0$, then either $\langle u, z \rangle > 0$ or $\langle u, z \rangle < 0$. In either case we show that we can find some point $z' \in C$ closer to $b$ than $z$ is, a contradiction.

Case 1: $\langle u, z \rangle > 0$.

Let $z' = (1 - \alpha)z$ for any $\alpha$ such that $0 < \alpha < 1$. Then $z' \in C$ and since $u = z - b$
\[
z' - b = (1 - \alpha)z - (z - u) = u - \alpha z,
\]
so
\[
\|z' - b\|^2 = \|u - \alpha z\|^2 = \|u\|^2 - 2\alpha \langle u, z \rangle + \alpha^2 \|z\|^2.
\]
If we pick $\alpha > 0$ such that $\alpha < 2\langle u, z \rangle / \|z\|^2$, then $-2\alpha \langle u, z \rangle + \alpha^2 \|z\|^2 < 0$, so $\|z' - b\|^2 < \|u\|^2 = \|z - b\|^2$, contradicting the fact that $z$ is a point of $C$ closest to $b$.

Case 2: $\langle u, z \rangle < 0$. 


11.1. VARIANTS OF THE FARKAS LEMMA

Let \( z' = (1 + \alpha)z \) for any \( \alpha \) such that \( \alpha \geq -1 \). Then \( z' \in C \) and since \( u = z - b \) we have

\[
\|z' - b\|^2 = \|u + \alpha z\|^2 = \|u\|^2 + 2\alpha \langle u, z \rangle + \alpha^2 \|z\|^2,
\]

and if

\[
0 < \alpha < -2\langle u, z \rangle / \|z\|^2,
\]

then \( 2\alpha \langle u, z \rangle + \alpha^2 \|z\|^2 < 0 \), so \( \|z' - b\|^2 < \|u\|^2 = \|z - b\|^2 \), a contradiction as above.

Therefore \( \langle u, z \rangle = 0 \). We have

\[
\langle u, u \rangle = \langle u, z - b \rangle = \langle u, z \rangle - \langle u, b \rangle = -\langle u, b \rangle,
\]

and since \( u \neq 0 \), we have \( \langle u, u \rangle > 0 \), so \( \langle u, u \rangle = -\langle u, b \rangle \) implies that

\[
\langle u, b \rangle < 0. \quad (\ast_2)
\]

It remains to prove that \( \langle u, a_i \rangle \geq 0 \) for \( i = 1, \ldots, m \). Pick any \( x \in C \) such that \( x \neq z \). We claim that

\[
\langle b - z, x - z \rangle \leq 0. \quad (\ast_3)
\]

Otherwise \( \langle b - z, x - z \rangle > 0 \), that is, \( \langle z - b, x - z \rangle < 0 \), and we show that we can find some point \( z' \in C \) on the line segment \([z, x]\) closer to \( b \) than \( z \) is.
For any \( \alpha \) such that \( 0 \leq \alpha \leq 1 \), we have \( z' = (1 - \alpha)z + \alpha x = z + \alpha(x - z) \in C \), and since \( z' - b = z - b + \alpha(x - z) \) we have
\[
\|z' - b\|^2 = \|z - b + \alpha(x - z)\|^2 = \|z - b\|^2 + 2\alpha \langle z - b, x - z \rangle + \alpha^2 \|x - z\|^2,
\]
so for any \( \alpha > 0 \) such that
\[
\alpha < -2\langle z - b, x - z \rangle / \|x - z\|^2,
\]
we have \( 2\alpha \langle z - b, x - z \rangle + \alpha^2 \|x - z\|^2 < 0 \), which implies that \( \|z' - b\|^2 < \|z - b\|^2 \), contradicting that \( z \) is a point of \( C \) closest to \( b \).

Since \( \langle b - z, x - z \rangle \leq 0 \), \( u = z - b \), and by \( (*)_1 \) \( \langle u, z \rangle = 0 \), we have
\[
0 \geq \langle b - z, x - z \rangle = \langle -u, x - z \rangle = \langle -u, x \rangle + \langle u, z \rangle = -\langle u, x \rangle,
\]
which means that
\[
\langle u, x \rangle \geq 0 \quad \text{for all } x \in C, \quad (*)_3
\]
as claimed. In particular,
\[
\langle u, a_i \rangle \geq 0 \quad \text{for } i = 1, \ldots, m. \quad (*)_4
\]
Then, by \( (*)_2 \) and \( (*)_4 \), the linear form defined by \( y = u^\top \) satisfies the properties \( yb < 0 \) and \( ya_i \geq 0 \) for \( i = 1, \ldots, m \), which proves the Farkas–Minkowski proposition.

There are other ways of proving the Farkas–Minkowski proposition, for instance using minimally infeasible systems or Fourier–Motzkin elimination; see Matousek and Gardner [73] (Chapter 6, Sections 6.6 and 6.7).

### 11.2 The Duality Theorem in Linear Programming

Let \( (P) \) be the linear program

\[
\text{maximize } cx \\
\text{subject to } Ax \leq b \text{ and } x \geq 0,
\]

with \( A \) a \( m \times n \) matrix, and assume that \( (P) \) has a feasible solution and is bounded above. Since by hypothesis the objective function \( x \mapsto cx \) is bounded on \( \mathcal{P}(A, b) \), it might be useful to deduce an upper bound for \( cx \) from the inequalities \( Ax \leq b \), for any \( x \in \mathcal{P}(A, b) \). We can do this as follows: for every inequality
\[
a_ix \leq b_i \quad 1 \leq i \leq m,
\]
pick a nonnegative scalar \( y_i \), multiply both sides of the above inequality by \( y_i \) obtaining
\[
y_ia_ix \leq y_ib_i \quad 1 \leq i \leq m,
\]
(the direction of the inequality is preserved since $y_i \geq 0$), and then add up these $m$ equations, which yields

$$(y_1 a_1 + \cdots + y_m a_m) x \leq y_1 b_1 + \cdots + y_m b_m.$$  

If we can pick the $y_i \geq 0$ such that

$$c \leq y_1 a_1 + \cdots + y_m a_m,$$

then since $x_j \geq 0$ we have

$$cx \leq (y_1 a_1 + \cdots + y_m a_m) x \leq y_1 b_1 + \cdots + y_m b_m,$$

namely we found an upper bound of the value $cx$ of the objective function of $(P)$ for any feasible solution $x \in \mathcal{P}(A,b)$. If we let $y$ be the linear form $y = (y_1, \ldots, y_m)$, then since

$$A = \begin{pmatrix} a_1 \\ \vdots \\ a_m \end{pmatrix}$$

$y_1 a_1 + \cdots + y_m a_m = yA$, and $y_1 b_1 + \cdots + y_m b_m = yb$, what we did was to look for some $y \in (\mathbb{R}^m)^*$ such that

$$c \leq yA, \quad y \geq 0,$$

so that we have

$$cx \leq yb \quad \text{for all } x \in \mathcal{P}(A,b).$$

Then it is natural to look for a “best” value of $yb$, namely a minimum value, which leads to the definition of the dual of the linear program $(P)$, a notion due to John von Neumann.

**Definition 11.1.** Given any linear program $(P)$

$$\begin{align*}
\text{maximize} & \quad cx \\
\text{subject to} & \quad Ax \leq b \text{ and } x \geq 0,
\end{align*}$$

with $A$ a $m \times n$ matrix, the dual $(D)$ of $(P)$ is the following optimization problem:

$$\begin{align*}
\text{minimize} & \quad yb \\
\text{subject to} & \quad yA \geq c \text{ and } y \geq 0,
\end{align*}$$

where $y \in (\mathbb{R}^m)^*$. The original linear program $(P)$ is called the primal linear program.

Here is an explicit example of a linear program and its dual.
Example 11.1. Consider the linear program illustrated by Figure 28.3

\[
\begin{align*}
\text{maximize} \quad & 2x_1 + 3x_2 \\
\text{subject to} \quad & 4x_1 + 8x_2 \leq 12 \\
& 2x_1 + x_2 \leq 3 \\
& 3x_1 + 2x_2 \leq 4 \\
& x_1 \geq 0, \quad x_2 \geq 0.
\end{align*}
\]

Its dual linear program is illustrated in Figure 28.2

\[
\begin{align*}
\text{minimize} \quad & 12y_1 + 3y_2 + 4y_3 \\
\text{subject to} \quad & 4y_1 + 2y_2 + 3y_3 \geq 2 \\
& 8y_1 + y_2 + 2y_3 \geq 3 \\
& y_1 \geq 0, \quad y_2 \geq 0, \quad y_3 \geq 0.
\end{align*}
\]

It can be checked that \((x_1, x_2) = (1/2, 5/4)\) is an optimal solution of the primal linear program, with the maximum value of the objective function \(2x_1 + 3x_2\) equal to \(19/4\), and that \((y_1, y_2, y_3) = (5/16, 0, 1/4)\) is an optimal solution of the dual linear program, with the minimum value of the objective function \(12y_1 + 3y_2 + 4y_3\) also equal to \(19/4\).

![Figure 11.2](image-url) - The \(\mathcal{H}\)-polytope for the linear program of Example 28.1. Note \(x_1 \rightarrow x\) and \(x_2 \rightarrow y\).

Observe that in the primal linear program \((P)\), we are looking for a vector \(x \in \mathbb{R}^n\) maximizing the form \(cx\), and that the constraints are determined by the action of the rows of the matrix \(A\) on \(x\). On the other hand, in the dual linear program \((D)\), we are looking
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Figure 11.3: The \( \mathcal{H} \)-polyhedron for the dual linear program of Example 28.1 is the spacial region “above” the pink plane and in “front” of the blue plane. Note \( y_1 \rightarrow x, y_2 \rightarrow y, \) and \( y_3 \rightarrow z. \)

for a linear form \( y \in (\mathbb{R}^*)^m \) minimizing the form \( yb, \) and the constraints are determined by the action of \( y \) on the columns of \( A. \) This is the sense in which \( (D) \) is the dual \( (P). \) In most presentations, the fact that \( (P) \) and \( (D) \) perform a search for a solution in spaces that are dual to each other is obscured by excessive use of transposition.

To convert the dual program \( (D) \) to a standard maximization problem we change the objective function \( yb \) to \( -b^\top y^\top \) and the inequality \( yA \geq c \) to \( -A^\top y^\top \leq -c^\top. \) The dual linear program \( (D) \) is now stated as \( (D') \)

\[
\text{maximize } \quad -b^\top y^\top \\
\text{subject to } \quad -A^\top y^\top \leq -c^\top \text{ and } y^\top \geq 0,
\]

where \( y \in (\mathbb{R}^m)^*. \) Observe that the dual in maximization form \( (D'') \) of the dual program \( (D') \) gives back the primal program \( (P). \)

The above discussion established the following inequality known as weak duality.

Proposition 11.6. (Weak Duality) Given any linear program \( (P) \)

\[
\text{maximize } \quad cx \\
\text{subject to } \quad Ax \leq b \text{ and } x \geq 0,
\]

with \( A \) a \( m \times n \) matrix, for any feasible solution \( x \in \mathbb{R}^n \) of the primal problem \( (P) \) and every feasible solution \( y \in (\mathbb{R}^m)^* \) of the dual problem \( (D), \) we have

\[
 cx \leq yb.
\]
We say that the dual linear program \((D)\) is bounded below if \(\{yb \mid y^\top \in \mathcal{P}(-A^\top, -c^\top)\}\) is bounded below.

What happens if \(x^*\) is an optimal solution of \((P)\) and if \(y^*\) is an optimal solution of \((D)\)? We have \(cx^* \leq y^*b\), but is there a “duality gap,” that is, is it possible that \(cx^* < y^*b\)?

The answer is no, this is the strong duality theorem. Actually, the strong duality theorem asserts more than this.

**Theorem 11.7. (Strong Duality for Linear Programming)** Let \((P)\) be any linear program

\[
\begin{align*}
\text{maximize} & \quad cx \\
\text{subject to} & \quad Ax \leq b \text{ and } x \geq 0,
\end{align*}
\]

with \(A\) a \(m \times n\) matrix. The primal problem \((P)\) has a feasible solution and is bounded above iff the dual problem \((D)\) has a feasible solution and is bounded below. Furthermore, if \((P)\) has a feasible solution and is bounded above, then for every optimal solution \(x^*\) of \((P)\) and every optimal solution \(y^*\) of \((D)\), we have

\[cx^* = y^*b.\]

**Proof.** If \((P)\) has a feasible solution and is bounded above then we know from Proposition 26.1 that \((P)\) has some optimal solution. Let \(x^*\) be any optimal solution of \((P)\). First we will show that \((D)\) has a feasible solution \(v\).

Let \(\mu = cx^*\) be the maximum of the objective function \(x \mapsto cx\). Then for any \(\epsilon > 0\), the system of inequalities

\[Ax \leq b, \quad x \geq 0, \quad cx \geq \mu + \epsilon\]

has no solution, since otherwise \(\mu\) would not be the maximum value of the objective function \(cx\). We would like to apply Farkas II, so first we transform the above system of inequalities into the system

\[
\begin{pmatrix} A \\ -c \end{pmatrix} x \leq \begin{pmatrix} b \\ -(\mu + \epsilon) \end{pmatrix}.
\]

By Proposition 28.3 (Farkas II), there is some linear form \((\lambda, z) \in (\mathbb{R}^{m+1})^*\) such that \(\lambda \geq 0, z \geq 0,\)

\[
(\lambda, z) \begin{pmatrix} A \\ -c \end{pmatrix} \geq 0_m^\top,
\]

and

\[
(\lambda, z) \begin{pmatrix} b \\ -(\mu + \epsilon) \end{pmatrix} < 0,
\]

which means that

\[\lambda A - zc \geq 0_m^\top, \quad \lambda b - z(\mu + \epsilon) < 0,\]
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that is,

\[ \lambda A \geq zc \]
\[ \lambda b < z(\mu + \epsilon) \]
\[ \lambda \geq 0, \ z \geq 0. \]

On the other hand, since \( x^* \geq 0 \) is an optimal solution of the system \( Ax \leq b \), by Farkas II again (by taking the negation of the equivalence), since \( \lambda A \geq 0 \) (for the same \( \lambda \) as before), we must have

\[ \lambda b \geq 0. \quad (\ast _1) \]

We claim that \( z > 0 \). Otherwise, since \( z \geq 0 \), we must have \( z = 0 \), but then

\[ \lambda b < z(\mu + \epsilon) \]

implies

\[ \lambda b < 0, \quad (\ast _2) \]

and since \( \lambda b \geq 0 \) by \( (\ast _1) \), we have a contradiction. Consequently, we can divide by \( z > 0 \) without changing the direction of inequalities, and we obtain

\[ \frac{\lambda}{z} A \geq c \]
\[ \frac{\lambda}{z} b < \mu + \epsilon \]
\[ \frac{\lambda}{z} \geq 0, \]

which shows that \( v = \lambda/z \) is a feasible solution of the dual problem \( (D) \). However, weak duality (Proposition 28.6) implies that \( cx^* = \mu \leq yb \) for any feasible solution \( y \geq 0 \) of the dual program \( (D) \), so \( (D) \) is bounded below and by Proposition 26.1 applied to the version of \( (D) \) written as a maximization problem, we conclude that \( (D) \) has some optimal solution. For any optimal solution \( y^* \) of \( (D) \), since \( v \) is a feasible solution of \( (D) \) such that \( vb < \mu + \epsilon \), we must have

\[ \mu \leq y^*b < \mu + \epsilon, \]

and since our reasoning is valid for any \( \epsilon > 0 \), we conclude that \( cx^* = \mu = y^*b \).

If we assume that the dual program \( (D) \) has a feasible solution and is bounded below, since the dual of \( (D) \) is \( (P) \), we conclude that \( (P) \) is also feasible and bounded above. \( \square \)

The strong duality theorem can also be proved by the simplex method, because when it terminates with an optimal solution of \( (P) \), the final tableau also produces an optimal solution \( y \) of \( (D) \) that can be read off the reduced costs of columns \( n + 1, \ldots, n + m \) by flipping their signs. We follow the proof in Ciarlet [30] (Chapter 10).
Theorem 11.8. Consider the linear program \((P)\),

$$\text{maximize } cx$$
$$\text{subject to } Ax \leq b \text{ and } x \geq 0,$$

its equivalent version \((P_2)\) in standard form,

$$\text{maximize } \hat{c} \hat{x}$$
$$\text{subject to } \hat{A}\hat{x} = b \text{ and } \hat{x} \geq 0,$$

where \(\hat{A}\) is an \(m \times (n + m)\) matrix, \(\hat{c}\) is a linear form in \((\mathbb{R}^{n+m})^*\), and \(\hat{x} \in \mathbb{R}^{n+m}\), given by

\[
\hat{A} = (A \ I_m), \quad \hat{c} = (c \ 0 \cdots)_m, \quad x = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix}, \quad \bar{x} = \begin{pmatrix} x_{n+1} \\ \vdots \\ x_{n+m} \end{pmatrix}, \quad \hat{x} = \begin{pmatrix} x \\ \bar{x} \end{pmatrix},
\]

and the dual \((D)\) of \((P)\) given by

$$\text{minimize } yb$$
$$\text{subject to } yA \geq c \text{ and } y \geq 0,$$

where \(y \in (\mathbb{R}^m)^*\). If the simplex algorithm applied to the linear program \((P_2)\) terminates with an optimal solution \((\hat{u}^*, K^*)\), where \(\hat{u}^*\) is a basic feasible solution and \(K^*\) is a basis for \(\hat{u}^*\), then \(y^* = \hat{c}_{K^*}\hat{A}_{K^*}^{-1}\) is an optimal solution for \((D)\) such that \(\hat{c}\hat{u}^* = y^*b\). Furthermore, \(y^*\) is given in terms of the reduced costs by \(y^* = -(\hat{c}_{K^*})_{n+1} \cdots (\hat{c}_{K^*})_{n+m}\).

Proof. We know that \(K^*\) is a subset of \(\{1, \ldots, n+m\}\) consisting of \(m\) indices such that the corresponding columns of \(\hat{A}\) are linearly independent. Let \(N^* = \{1, \ldots, n+m\} - K^*\). The simplex methods terminates with an optimal solution in Case (A), namely when

$$\hat{c}_j - \sum_{k \in K} \gamma_k^j \hat{c}_k \leq 0 \quad \text{for all } j \in N^*,$$

where \(\hat{A}_j = \sum_{k \in K^*} \gamma_k^j \hat{A}_k\), or using the notations of Section 27.3,

$$\hat{c}_j - \hat{c}_{K^*}\hat{A}_{K^*}^{-1}\hat{A}_j \leq 0 \quad \text{for all } j \in N^*.$$

The above inequalities can be written as

$$\hat{c}_{N^*} - \hat{c}_{K^*}\hat{A}_{K^*}^{-1}\hat{A}_{N^*} \leq 0_{n^*},$$

or equivalently as

$$\hat{c}_{K^*}\hat{A}_{K^*}^{-1}\hat{A}_{N^*} \geq \hat{c}_{N^*}. \quad (\because_1)$$
The value of the objective function for the optimal solution $\hat{u}^*$ is $\hat{c}\hat{u}^* = \hat{c}_{K^*}\hat{u}_{K^*}$, and since $\hat{u}_{K^*}$ satisfies the equation $\hat{A}_{K^*}\hat{u}_{K^*} = b$, the value of the objective function is

$$\hat{c}_{K^*}\hat{u}_{K^*} = \hat{c}_{K^*}\hat{A}_{K^*}^{-1}b. \quad (*)_2$$

Then if we let $y^* = \hat{c}_{K^*}\hat{A}_{K^*}^{-1}$, obviously we have $y^*b = \hat{c}_{K^*}\hat{u}_{K^*}$, so if we can prove that $y^*$ is a feasible solution of the dual linear program $(D)$, by weak duality, $y^*$ is an optimal solution of $(D)$. We have

$$y^*\hat{A}_{K^*} = \hat{c}_{K^*}\hat{A}_{K^*}^{-1}\hat{A}_{K^*} = \hat{c}_{K^*}, \quad (*)_3$$

and by $(*)_1$ we get

$$y^*\hat{A}_{N^*} = \hat{c}_{K^*}\hat{A}_{K^*}^{-1}\hat{A}_{N^*} \geq \hat{c}_{N^*}. \quad (*)_4$$

Let $P$ be the $(n + m) \times (n + m)$ permutation matrix defined so that

$$\hat{A}P = (A \ I_m) P = (\hat{A}_{K^*} \ \hat{A}_{N^*}).$$

Then we also have

$$\hat{c}P = (c \ 0^T_m) P = (c_{K^*} \ c_{N^*}).$$

Using the equations $(*)_3$ and $(*)_4$ we obtain

$$y^*\left(\hat{A}_{K^*} \ \hat{A}_{N^*}\right) \geq \left(c_{K^*} \ c_{N^*}\right),$$

that is,

$$y^*(A \ I_m) \geq (c \ 0^T_m),$$

which is equivalent to

$$y^*(A \ I_m) \geq (c \ 0^T_m),$$

that is

$$y^*A \geq c, \quad y \geq 0,$$

and these are exactly the conditions that say that $y^*$ is a feasible solution of the dual program $(D)$.

The reduced costs are given by $(\hat{c}_{K^*})_i = \hat{c}_i - \hat{c}_{K^*}\hat{A}_{K^*}^{-1}\hat{A}_i$, for $i = 1, \ldots, n + m$. But for $i = n + 1, \ldots, n + m$ each column $\hat{A}_{n+j}$ is the $j$th vector of the identity matrix $I_m$, so

$$(\hat{c}_{K^*})_{n+j} = -\hat{c}_{K^*}\hat{A}_{K^*}^{-1}_{n+j} = -y^*_j \quad j = 1, \ldots, m,$$

as claimed. \qed

The fact that the above proof is fairly short is deceptive, because this proof relies on the fact that there are versions of the simplex algorithm using pivot rules that prevent cycling, but the proof that such pivot rules work correctly is quite lengthy. Other proofs are given
in Matousek and Gardner [73] (Chapter 6, Sections 6.3), Chvatal [29] (Chapter 5), and Papadimitriou and Steiglitz [80] (Section 2.7).

Observe that since the last \( m \) rows of the final tableau are actually obtained by multiplying \([u \hat{A}]\) by \( \hat{A}_K^{-1} \), the \( m \times m \) matrix consisting of the last \( m \) columns and last \( m \) rows of the final tableau is \( \hat{A}_K^{-1} \) (basically, the simplex algorithm has performed the steps of a Gauss–Jordan reduction). This fact allows saving some steps in the primal dual method.

By combining weak duality and strong duality, we obtain the following theorem which shows that exactly four cases arise.

**Theorem 11.9.** (Duality Theorem of Linear Programming) Let \((P)\) be any linear program

\[
\text{maximize} \quad cx \\
\text{subject to} \quad Ax \leq b \text{ and } x \geq 0,
\]

and let \((D)\) be its dual program

\[
\text{minimize} \quad yb \\
\text{subject to} \quad yA \geq c \text{ and } y \geq 0,
\]

with \( A \) a \( m \times n \) matrix. Then exactly one of the following possibilities occur:

1. Neither \((P)\) nor \((D)\) has a feasible solution.
2. \((P)\) is unbounded and \((D)\) has no feasible solution.
3. \((P)\) has no feasible solution and \((D)\) is unbounded.
4. Both \((P)\) and \((D)\) have a feasible solution. Then both have an optimal solution, and for every optimal solution \( x^* \) of \((P)\) and every optimal solution \( y^* \) of \((D)\), we have

\[
-cx^* = y^*b.
\]

An interesting corollary of Theorem 28.9 is that there is a test to determine whether a linear program \((P)\) has an optimal solution. Indeed, \((P)\) has an optimal solution iff the following set of constraints is satisfiable:

\[
\begin{align*}
Ax & \leq b \\
yA & \geq c \\
-cx & \geq yb \\
x & \geq 0, \ y \geq 0_m^\top.
\end{align*}
\]

In fact, for any feasible solution \((x^*, y^*)\) of the above system, \(x^*\) is an optimal solution of \((P)\) and \(y^*\) is an optimal solution of \((D)\)
11.3 Complementary Slackness Conditions

Another useful corollary of the strong duality theorem is the following result known as the equilibrium theorem.

**Theorem 11.10. (Equilibrium Theorem)** For any linear program \((P)\) and its dual linear program \((D)\) (with set of inequalities \(Ax \leq b\) where \(A\) is an \(m \times n\) matrix, and objective function \(x \mapsto cx\)), for any feasible solution \(x\) of \((P)\) and any feasible solution \(y\) of \((D)\), \(x\) and \(y\) are optimal solutions iff

\[
y_i = 0 \quad \text{for all } i \text{ for which } \sum_{j=1}^{n} a_{ij} x_j < b_i \quad (\ast_D)
\]

and

\[
x_j = 0 \quad \text{for all } j \text{ for which } \sum_{i=1}^{m} y_i a_{ij} > c_j. \quad (\ast_P)
\]

**Proof.** First, assume that \((\ast_D)\) and \((\ast_P)\) hold. The equations in \((\ast_D)\) say that \(y_i = 0\) unless \(\sum_{j=1}^{n} a_{ij} x_j = b_i\), hence

\[
yb = \sum_{i=1}^{m} y_i b_i = \sum_{i=1}^{m} y_i \sum_{j=1}^{n} a_{ij} x_j = \sum_{i=1}^{m} \sum_{j=1}^{n} y_i a_{ij} x_j.
\]

Similarly, the equations in \((\ast_P)\) say that \(x_j = 0\) unless \(\sum_{i=1}^{m} y_i a_{ij} = c_j\), hence

\[
cx = \sum_{j=1}^{n} c_j x_j = \sum_{j=1}^{n} \sum_{i=1}^{m} y_i a_{ij} x_j.
\]

Consequently, we obtain

\[
cx = yb.
\]

By weak duality (Proposition 28.6), we have

\[
cx \leq yb = cx
\]

for all feasible solutions \(x\) of \((P)\), so \(x\) is an optimal solution of \((P)\). Similarly,

\[
yb = cx \leq yb
\]

for all feasible solutions \(y\) of \((D)\), so \(y\) is an optimal solution of \((D)\).

Let us now assume that \(x\) is an optimal solution of \((P)\) and that \(y\) is an optimal solution of \((D)\). Then, as in the proof of Proposition 28.6,

\[
\sum_{j=1}^{n} c_j x_j \leq \sum_{i=1}^{m} \sum_{j=1}^{n} y_i a_{ij} x_j \leq \sum_{i=1}^{m} y_i b_i.
\]
By strong duality, since $x$ and $y$ are optimal solutions the above inequalities are actually equalities, so in particular we have

$$\sum_{j=1}^{n} \left( c_j - \sum_{i=1}^{m} y_i a_{ij} \right) x_j = 0.$$ 

Since $x$ and $y^*$ are feasible, $x_i \geq 0$ and $y_j \geq 0$, so if $\sum_{i=1}^{m} y_i a_{ij} > c_j$, we must have $x_j = 0$. Similarly, we have

$$\sum_{i=1}^{m} y_i \left( \sum_{j=1}^{m} a_{ij} x_j - b_i \right) = 0,$$

so if $\sum_{j=1}^{m} a_{ij} x_j < b_i$, then $y_i = 0$. \hfill \square

The equations in $(\ast_p)$ and $(\ast_P)$ are often called complementary slackness conditions. These conditions can be exploited to solve for an optimal solution of the primal problem with the help of the dual problem, and conversely. Indeed, if we guess a solution to one problem, then we may solve for a solution of the dual using the complementary slackness conditions, and then check that our guess was correct. This is the essence of the primal-dual methods. To present this method, first we need to take a closer look at the dual of a linear program already in standard form.

### 11.4 Duality for Linear Programs in Standard Form

Let $(P)$ be a linear program in standard form, where $Ax = b$ for some $m \times n$ matrix of rank $m$ and some objective function $x \mapsto cx$ (of course, $x \geq 0$). To obtain the dual of $(P)$ we convert the equations $Ax = b$ to the following system of inequalities involving a $(2m) \times n$ matrix.

$$\begin{pmatrix} A \\ -A \end{pmatrix} x \leq \begin{pmatrix} b \\ -b \end{pmatrix}.$$

Then, if we denote the $2m$ dual variables by $(y', y'')$, with $y', y'' \in (\mathbb{R}^m)^*$, the dual of the above program is

\[
\begin{align*}
\text{minimize} & \quad y'b - y''b \\
\text{subject to} & \quad (y', y'') \begin{pmatrix} A \\ -A \end{pmatrix} \geq c \text{ and } y', y'' \geq 0,
\end{align*}
\]

where $y', y'' \in (\mathbb{R}^m)^*$, which is equivalent to

\[
\begin{align*}
\text{minimize} & \quad (y' - y'')b \\
\text{subject to} & \quad (y' - y'')A \geq c \text{ and } y', y'' \geq 0,
\end{align*}
\]
where \( y', y'' \in (\mathbb{R}^m)^* \). If we write \( y = y' - y'' \), we find that the above linear program is equivalent to the following linear program \((D)\):

\[
\begin{align*}
\text{minimize} & \quad yb \\
\text{subject to} & \quad yA \geq c,
\end{align*}
\]

where \( y \in (\mathbb{R}^m)^* \). Observe that \( y \) is not required to be nonnegative; it is arbitrary.

Next, we would like to know what is the version of Theorem 28.8 for a linear program already in standard form. This is very simple.

**Theorem 11.11.** Consider the linear program \((P2)\) in standard form

\[
\begin{align*}
\text{maximize} & \quad cx \\
\text{subject to} & \quad Ax = b \text{ and } x \geq 0,
\end{align*}
\]

and its dual \((D)\) given by

\[
\begin{align*}
\text{minimize} & \quad yb \\
\text{subject to} & \quad yA \geq c,
\end{align*}
\]

where \( y \in (\mathbb{R}^m)^* \). If the simplex algorithm applied to the linear program \((P2)\) terminates with an optimal solution \((u^*, K^*)\), where \( u^* \) is a basic feasible solution and \( K^* \) is a basis for \( u^* \), then \( y^* = c_{K^*}A_{K^*}^{-1} \) is an optimal solution for \((D)\) such that \( cu^* = y^* b \). Furthermore, if we assume that the simplex algorithm is started with a basic feasible solution \((u_0, K_0)\) where \( K_0 = (n - m + 1, \ldots, n) \) (the indices of the last \( m \) columns of \( A \)) and \( A_{(n-m+1,\ldots,n)} = I_m \) (the last \( m \) columns of \( A \) constitute the identity matrix \( I_m \)), then the optimal solution \( y^* = c_{K^*}A_{K^*}^{-1} \) for \((D)\) is given in terms of the reduced costs by

\[
y^* = c_{(n-m+1,\ldots,n)} - (c_{K^*})_{(n-m+1,\ldots,n)},
\]

and the \( m \times m \) matrix consisting of last \( m \) columns and the last \( m \) rows of the final tableau is \( A_{K^*}^{-1} \).

**Proof.** The proof of Theorem 28.8 applies with \( A \) instead of \( \hat{A} \) and we can show that

\[
c_{K^*}A_{K^*}^{-1}A_{N^*} \geq c_{N^*},
\]

and that \( y^* = c_{K^*}A_{K^*}^{-1} \) satisfies, \( cu^* = y^* b \), and

\[
\begin{align*}
y^*A_{K^*} & = c_{K^*}A_{K^*}^{-1}A_{K^*} = c_{K^*}, \\
y^*A_{N^*} & = c_{K^*}A_{K^*}^{-1}A_{N^*} \geq c_{N^*}.
\end{align*}
\]

Let \( P \) be the \( n \times n \) permutation matrix defined so that

\[
AP = (A_{K^*} A_{N^*}).
\]
Then we also have
\[ c^P = (c_{K^*} \quad c_{N^*}), \]
and using the above equations and inequalities we obtain
\[ y^*(A_{K^*} \quad A_{N^*}) \geq (c_{K^*} \quad c_{N^*}), \]
that is, \( y^*A^P \geq c^P \), which is equivalent to
\[ y^*A \geq c, \]
which shows that \( y^* \) is a feasible solution of \((D)\) (remember, \( y^* \) is arbitrary so there is no need for the constraint \( y^* \geq 0 \)).

The reduced costs are given by
\[
(c_{K^*})_i = c_i - c_{K^*}A_{K^*}^{-1}A_i,
\]
and since for \( j = n - m + 1, \ldots, n \) the column \( A^j \) is the \((j + m - n)\)th column of the identity matrix \( I_m \), we have
\[
(c_{K^*})_j = c_j - (c_{K^*}A_{K^*})_{j+m-n}, \quad j = n - m + 1, \ldots, n,
\]
that is,
\[ y^* = c_{(n-m+1,...,n)} - (c_{K^*})_{(n-m+1,...,n)}, \]
as claimed. Since the last \( m \) rows of the final tableau is obtained by multiplying \([u_0 \ A]\) by \( A_{K^*}^{-1} \), and the last \( m \) columns of \( A \) constitute \( I_m \), the last \( m \) rows and the last \( m \) columns of the final tableau constitute \( A_{K^*}^{-1} \).

Let us now take a look at the complementary slackness conditions of Theorem 28.10. If we go back to the version of \((P)\) given by
\[
\begin{align*}
\text{maximize} \quad & cx \\
\text{subject to} \quad & (A \begin{bmatrix} x \end{bmatrix} \begin{bmatrix} b \\ -b \end{bmatrix}) \quad \text{and} \quad x \geq 0,
\end{align*}
\]
and to the version of \((D)\) given by
\[
\begin{align*}
\text{minimize} \quad & y^'b - y^''b \\
\text{subject to} \quad & (y^' \begin{bmatrix} y^'' \end{bmatrix}) \begin{bmatrix} A \\ -A \end{bmatrix} \quad \text{and} \quad y^', y^'' \geq 0,
\end{align*}
\]
where \( y^', y^'' \in (\mathbb{R}^m)^* \), since the inequalities \( Ax \leq b \) and \( -Ax \leq -b \) together imply that \( Ax = b \), we have equality for all these inequality constraints, and so the Conditions \((*D)\) place no constraints at all on \( y^' \) and \( y^'' \), while the Conditions \((*P)\) assert that
\[ x_j = 0 \quad \text{for all} \quad j \quad \text{for which} \quad \sum_{i=1}^{m} (y^'_i - y^''_i)a_{ij} > c_j. \]
If we write \( y = y' - y'' \), the above conditions are equivalent to
\[
x_j = 0 \quad \text{for all } j \text{ for which } \sum_{i=1}^{m} y_i a_{ij} > c_j.
\]
Thus we have the following version of Theorem 28.10.

**Theorem 11.12.** (Equilibrium Theorem, Version 2) For any linear program \((P_2)\) in standard form (with set of equalities \(Ax \leq b\) where \(A\) is an \(m \times n\) matrix, and objective function \(x \mapsto cx\)) and its dual linear program \((D)\), for any feasible solution \(x\) of \((P)\) and any feasible solution \(y\) of \((D)\), \(x\) and \(y\) are optimal solutions iff
\[
x_j = 0 \quad \text{for all } j \text{ for which } \sum_{i=1}^{m} y_i a_{ij} > c_j.
\]

\((*)_P\)

Therefore, the slackness conditions applied to a linear program \((P_2)\) in standard form and to its dual \((D)\) only impose slackness conditions on the variables \(x_j\) of the primal problem.

The above fact plays a crucial role in the primal-dual method.

### 11.5 The Dual Simplex Algorithm

Given a linear program \((P_2)\) in standard form
\[
\begin{align*}
\text{maximize} & \quad cx \\
\text{subject to} & \quad Ax = b \text{ and } x \geq 0,
\end{align*}
\]
where \(A\) is an \(m \times n\) matrix of rank \(m\), if no obvious feasible solution is available but if \(c \leq 0\), then rather than using the method for finding a feasible solution described in Section 27.2 we may use a method known as the dual simplex algorithm. This method uses basic solutions \((u, K)\) where \(Au = b\) and \(u_j = 0\) for all \(u_j \notin K\), but does not require \(u \geq 0\), so \(u\) may not be feasible. However, \(y = c_K A_K^{-1}\) is required to be feasible for the dual program
\[
\begin{align*}
\text{minimize} & \quad yb \\
\text{subject to} & \quad yA \geq c,
\end{align*}
\]
where \(y \in (\mathbb{R}^*)^m\). Since \(c \leq 0\), observe that \(y = 0^+_m\) is a feasible solution of the dual.

If a basic solution \(u\) of \((P_2)\) is found such that \(u \geq 0\), then \(cu = yb\) for \(y = c_K A_K^{-1}\), and we have found an optimal solution \(u\) for \((P_2)\) and \(y\) for \((D)\). The dual simplex method makes progress by attempting to make negative components of \(u\) zero and by decreasing the objective function of the dual program.

The dual simplex method starts with a basic solution \((u, K)\) of \(Ax = b\) which is not feasible but for which \(y = c_K A_K^{-1}\) is dual feasible. In many cases, the original linear program is specified by a set of inequalities \(Ax \leq b\) with some \(b_i < 0\), so by adding slack variables it is
easy to find such basic solution \( u \), and if in addition \( c \leq 0 \), then because the cost associated with slack variables is 0, we see that \( y = 0 \) is a feasible solution of the dual.

Given a basic solution \((u, K)\) of \( Ax = b \) (feasible or not), \( y = c_K A_K^{-1} \) is dual feasible iff \( c_K A_K^{-1} A \geq c \), and since \( c_K A_K^{-1} A_K = c_K \), the inequality \( c_K A_K^{-1} A \geq c \) is equivalent to \( c_K A_K^{-1} A_N \geq c_N \), that is,

\[
c_N - c_K A_K^{-1} A_N \leq 0,
\]

where \( N = \{1, \ldots, n\} - K \). Equation \((*)_1\) is equivalent to

\[
c_j - c_K \gamma^j_K \leq 0 \quad \text{for all } j \in N,
\]

where \( \gamma^j_K = A_K^{-1} A^j \). Recall that the notation \( \tilde{\gamma} \) is used to denote \( c_j - c_K \gamma^j_K \), which is called the reduced cost of the variable \( x_j \).

As in the simplex algorithm we need to decide which column \( A^k \) leaves the basis \( K \) and which column \( A^j \) enters the new basis \( K^+ \), in such a way that \( y^+ = c_K A_K^{-1} \) is a feasible solution of \((D)\), that is,

\[
c_N^+ - c_K A_K^{-1} A_N^+ \leq 0,
\]

where \( N^+ = \{1, \ldots, n\} - K^+ \). We use Proposition 27.2 to decide which column \( k^- \) should leave the basis.

Suppose \((u, K)\) is a solution of \( Ax = b \) for which \( y = c_K A_K^{-1} \) is dual feasible.

**Case (A).** If \( u \geq 0 \), then \( u \) is an optimal solution of \((P2)\).

**Case (B).** There is some \( k \in K \) such that \( u_k < 0 \). In this case, pick some \( k^- \in K \) such that \( u_{k^-} < 0 \) (according to some pivot rule).

**Case (B1).** Suppose that \( \gamma^j_{k^-} \geq 0 \) for all \( j \notin K \) (in fact, for all \( j \), since \( \gamma^j_{k^-} \in \{0,1\} \) for all \( j \in K \)). If so, we we claim that \((P2)\) is not feasible.

Indeed, let \( v \) be some basic feasible solution. We have \( v \geq 0 \) and \( Av = b \), that is,

\[
\sum_{j=1}^{n} v_j A^j = b,
\]

so by multiplying both sides by \( A_K^{-1} \) and using the fact that by definition \( \gamma^j_K = A_K^{-1} A^j \), we obtain

\[
\sum_{j=1}^{n} v_j \gamma^j_K = A_K^{-1} b = u_K.
\]

But recall that by hypothesis \( u_{k^-} < 0 \), yet \( v_j \geq 0 \) and \( \gamma^j_{k^-} \geq 0 \) for all \( j \), so the component of index \( k^- \) is zero or positive on the left, and negative on the right, a contradiction. Therefore, \((P2)\) is indeed not feasible.

**Case (B2).** We have \( \gamma^j_{k^-} < 0 \) for some \( j \).

We pick the column \( A^j \) entering the basis among those for which \( \gamma^j_{k^-} < 0 \). Since we assumed that \( c_j - c_K \gamma^j_K \leq 0 \) for all \( j \in N \) by \((*)_2\), consider

\[
\mu^+ = \max \left\{ \frac{c_j - c_K \gamma^j_K}{\gamma^j_{k^-}} \mid \gamma^j_{k^-} < 0, \ j \in N \right\} = \max \left\{ -\frac{\tilde{\gamma}^j_j}{\gamma^j_{k^-}} \mid \gamma^j_{k^-} < 0, \ j \in N \right\} \leq 0,
\]
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and the set

\[ N(\mu^+) = \left\{ j \in N \mid \frac{c_j}{\gamma_j^+} = \mu^+ \right\}. \]

We pick some index \( j^+ \in N(\mu^+) \) as the index of the column entering the basis (using some pivot rule).

Recall that by hypothesis \( c_i - c_K \gamma_i^j \leq 0 \) for all \( j \notin K \) and \( c_i - c_K \gamma_i^+_K = 0 \) for all \( i \in K \). Since \( \gamma_k^+ < 0 \), for any index \( j \) such that \( \gamma_i^j \geq 0 \), we have \( -\gamma_i^j / \gamma_j^+ \geq 0 \), and since by Proposition 27.2

\[ c_i - c_K \gamma_i^j = c_i - c_K \gamma_i^+ \gamma_i^j - \frac{\gamma_i^j}{\gamma_j^+} (c_j^+ - c_K \gamma_i^j), \]

we have \( c_i - c_K \gamma_i^j \leq 0 \). For any index \( i \) such that \( \gamma_i^j < 0 \), by the choice of \( j^+ \in K^* \),

\[ \frac{c_i - c_K \gamma_i^j}{\gamma_i^j} \leq \frac{c_j^+ - c_K \gamma_j^+}{\gamma_j^+}, \]

so

\[ c_i - c_K \gamma_i^j - \frac{\gamma_i^j}{\gamma_j^+} (c_j^+ - c_K \gamma_j^+) \leq 0, \]

and again, \( c_i - c_K \gamma_i^j \leq 0 \). Therefore, if we let \( K^+ = (K - \{k^-\}) \cup \{j^+\} \), then \( y^+ = c_K A_{K^+}^{-1} \) is dual feasible. As in the simplex algorithm, \( \theta^+ \) is given by

\[ \theta^+ = u_{k^-} / \gamma_{k^-}^+ \geq 0, \]

and \( u^+ \) is also computed as in the simplex algorithm by

\[ u_i^+ = \begin{cases} u_i - \theta^+ \gamma_i^+ & \text{if } i \in K \\ \theta^+ & \text{if } i = j^+ \\ 0 & \text{if } i \notin K \cup \{j^+\} \end{cases}. \]

The change in the objective function of the prime and dual program (which is the same, since \( u_K = A_{K^+}^{-1} b \) and \( y = c_K A_{K^+}^{-1} \) is chosen such that \( cu = c_K u_K = yb \)) is the same as in the simplex algorithm, namely

\[ \theta^+ (c_j^+ - c_K \gamma_j^+). \]

We have \( \theta^+ > 0 \) and \( c_j^+ - c_K \gamma_j^+ \leq 0 \), so if \( c_j^+ - c_K \gamma_j^+ < 0 \), then the objective function of the dual program decreases strictly.

**Case (B3).** \( \mu^+ = 0 \).

The possibility that \( \mu^+ = 0 \), that is, \( c_j^+ - c_K \gamma_j^+ = 0 \), may arise. In this case, the objective function doesn’t change. This is a case of degeneracy similar to the degeneracy that arises in the simplex algorithm. We still pick \( j^+ \in N(\mu^+) \), but we need a pivot rule that prevents
cycling. Such rules exist; see Bertsimas and Tsitsiklis [17] (Section 4.5) and Papadimitriou and Steiglitz [80] (Section 3.6).

The reader surely noticed that the dual simplex algorithm is very similar to the simplex algorithm, except that the simplex algorithm preserves the property that \((u, K)\) is (primal) feasible, whereas the dual simplex algorithm preserves the property that \(y = c_K A_K^{-1}\) is dual feasible. One might then wonder whether the dual simplex algorithm is equivalent to the simplex algorithm applied to the dual problem. This is indeed the case, there is a one-to-one correspondence between the dual simplex algorithm and the simplex algorithm applied to the dual problem. This correspondence is described in Papadimitriou and Steiglitz [80] (Section 3.7).

The comparison between the simplex algorithm and the dual simplex algorithm is best illustrated if we use a description of these methods in terms of (full) tableaux.

Recall that a (full) tableau is an \((m + 1) \times (n + 1)\) matrix organized as follows:

\[
\begin{array}{cccc}
-c_K u_K & \bar{c}_1 & \cdots & \bar{c}_j & \cdots & \bar{c}_n \\
 u_{k_1} & \gamma^1_1 & \cdots & \gamma^j_1 & \cdots & \gamma^n_1 \\
 \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\
 u_{k_m} & \gamma^1_m & \cdots & \gamma^j_m & \cdots & \gamma^n_m \\
\end{array}
\]

The top row contains the current value of the objective function and the reduced costs, the first column except for its top entry contain the components of the current basic solution \(u_K\), and the remaining columns except for their top entry contain the vectors \(\gamma^j_k\). Observe that the \(\gamma^j_K\) corresponding to indices \(j \in K\) constitute a permutation of the identity matrix \(I_m\). A tableau together with the new basis \(K^+ = (K - \{k^-\}) \cup \{j^+\}\) contains all the data needed to compute the new \(u_{K^+}\), the new \(\gamma^j_{K^+}\), and the new reduced costs \(\bar{c}_i - (\gamma^i_{k^-} / \gamma^j_{k^-}) \bar{c}_{j^+}\).

When executing the simplex algorithm, we have \(u_k \geq 0\) for all \(k \in K\) (and \(u_j = 0\) for all \(j \notin K\)), and the incoming column \(j^+\) is determined by picking one of the column indices such that \(\bar{c}_j > 0\). Then, the index \(k^-\) of the leaving column is determined by looking at the minimum of the ratios \(u_k / \gamma^j_k\) for which \(\gamma^j_k > 0\) (along column \(j^+\)).

On the other hand, when executing the dual simplex algorithm, we have \(\bar{c}_j \leq 0\) for all \(j \notin K\) (and \(\bar{c}_k = 0\) for all \(k \in K\)), and the outgoing column \(k^-\) is determined by picking one of the row indices such that \(u_k < 0\). The index \(j^+\) of the incoming column is determined by looking at the maximum of the ratios \(-\bar{c}_j / \gamma^j_k\) for which \(\gamma^j_k < 0\) (along row \(k^-\)).

More details about the comparison between the simplex algorithm and the dual simplex algorithm can be found in Bertsimas and Tsitsiklis [17] and Papadimitriou and Steiglitz [80].

Here is an example of the the dual simplex method.
Example 11.2. Consider the following linear program in standard form:

Maximize \(-4x_1 - 2x_2 - x_3\)

subject to

\[
\begin{pmatrix}
-1 & -1 & 2 & 1 & 0 & 0 \\
-4 & -2 & 1 & 0 & 1 & 0 \\
1 & 1 & -4 & 0 & 0 & 1
\end{pmatrix}
\begin{pmatrix}
x_1 \\
x_2 \\
x_3 \\
x_4 \\
x_5 \\
x_6
\end{pmatrix}
= \begin{pmatrix}
-3 \\
-4 \\
2
\end{pmatrix}
\]

and \((x_1, x_2, x_3, x_4, x_5, x_6) \geq 0\).

We initialize the dual simplex procedure with \((u, K)\) where

\[
\begin{pmatrix}
0 \\
0 \\
-3 \\
-4 \\
1
\end{pmatrix}
\]

and \(K = (4, 5, 6)\).

The initial tableau, before explicitly calculating the reduced cost, is

\[
\begin{array}{cccccc|c}
0 & \bar{c}_1 & \bar{c}_2 & \bar{c}_3 & \bar{c}_4 & \bar{c}_5 & \bar{c}_6 \\
\hline
u_4 = -3 & -1 & -1 & 2 & 1 & 0 & 0 \\
u_5 = -4 & -4 & -2 & 1 & 0 & 1 & 0 \\
u_6 = 2 & 1 & 1 & -4 & 0 & 0 & 1
\end{array}
\]

Since \(u\) has negative coordinates, Case (B) applies, and we will set \(k^- = 4\). We must now determine whether Case (B1) or Case (B2) applies. This determination is accomplished by scanning the first three columns in the tableau, and observing each column has a negative entry. Thus Case (B2) is applicable, and we need to determine the reduced costs. Observe that \(c = (-4, -2, -1, 0, 0, 0)\), which in turn implies \(c_{(4,5,6)} = (0,0,0)\). Equation \((*)_2\) implies that the nonzero reduced costs are

\[
\begin{align*}
\bar{c}_1 &= c_1 - c_{(4,5,6)} \\
&= \begin{pmatrix}
-4 \\
1
\end{pmatrix} \\
&= -4 \\
\bar{c}_2 &= c_2 - c_{(4,5,6)} \\
&= \begin{pmatrix}
-2 \\
1
\end{pmatrix} \\
&= -2 \\
\bar{c}_3 &= c_3 - c_{(4,5,6)} \\
&= \begin{pmatrix}
1 \\
4
\end{pmatrix} \\
&= -1,
\end{align*}
\]

and our tableau becomes

\[
\begin{array}{cccccc|c}
0 & -4 & -2 & -1 & 0 & 0 & 0 \\
\hline
u_4 = -3 & -1 & -1 & 2 & 1 & 0 & 0 \\
u_5 = -4 & -4 & -2 & 1 & 0 & 1 & 0 \\
u_6 = 2 & 1 & 1 & -4 & 0 & 0 & 1
\end{array}
\]
Since \( k^- = 4 \), our pivot row is the first row of the tableau. To determine candidates for \( j^+ \), we scan this row, locate negative entries and compute

\[
\mu^+ = \max \left\{ \frac{-c_j}{\gamma_j^+} \mid \gamma_j^+ < 0, \ j \in \{1, 2, 3\} \right\} = \max \left\{ \frac{-2}{1}, \frac{-4}{1} \right\} = -2.
\]

Since \( \mu^+ \) occurs when \( j = 2 \), we set \( j^+ = 2 \). Our new basis is \( K^+ = (2, 5, 6) \). We must normalize the first row of the tableau, namely multiply by \(-1\), then add twice this normalized row to the second row, and subtract the normalized row from the third row to obtain the updated tableau.

\[
\begin{array}{ccccccc}
0 & -4 & -2 & -1 & 0 & 0 & 0 \\
u_2 = 3 & 1 & 1 & -2 & -1 & 0 & 0 \\
u_5 = 2 & -2 & 0 & -3 & -2 & 1 & 0 \\
u_6 = -1 & 0 & 0 & -2 & 1 & 0 & 1 \\
\end{array}
\]

It remains to update the reduced costs and the value of the objective function by adding twice the normalized row to the top row.

\[
\begin{array}{ccccccc}
6 & -2 & 0 & -5 & -2 & 0 & 0 \\
u_2 = 3 & 1 & 1 & -2 & -1 & 0 & 0 \\
u_5 = 2 & -2 & 0 & -3 & -2 & 1 & 0 \\
u_6 = -1 & 0 & 0 & -2 & 1 & 0 & 1 \\
\end{array}
\]

We now repeat the procedure of Case (B2) and set \( k^- = 6 \) (since this is the only negative entry of \( u^+ \)). Our pivot row is now the third row of the updated tableaux, and the new \( \mu^+ \) becomes

\[
\mu^+ = \max \left\{ \frac{-c_j}{\gamma_j^+} \mid \gamma_j^+ < 0, \ j \in \{1, 3, 4\} \right\} = \max \left\{ \frac{-5}{2} \right\} = -\frac{5}{2},
\]

which implies that \( j^+ = 3 \). Hence the new basis is \( K^+ = (2, 5, 3) \), and we update the tableau by taking \(-\frac{1}{2}\) of Row 3, adding twice the normalized Row 3 to Row 1, and adding three times the normalized Row 3 to Row 2.

\[
\begin{array}{ccccccc}
6 & -2 & 0 & -5 & -2 & 0 & 0 \\
u_2 = 4 & 1 & 1 & 0 & -2 & 0 & -1 \\
u_5 = 7/2 & -2 & 0 & 0 & -7/2 & 1 & -3/2 \\
u_3 = 1/2 & 0 & 0 & 1 & -1/2 & 0 & -1/2 \\
\end{array}
\]

It remains to update the objective function and the reduced costs by adding five times the normalized row to the top row.

\[
\begin{array}{ccccccc}
17/2 & -2 & 0 & 0 & -9/2 & 0 & -5/2 \\
u_2 = 4 & 1 & 1 & 0 & -2 & 0 & -1 \\
u_5 = 7/2 & -2 & 0 & 0 & -7/2 & 1 & -3/2 \\
u_3 = 1/2 & 0 & 0 & 1 & -1/2 & 0 & -1/2 \\
\end{array}
\]

Since \( u^+ \) has no negative entries, the dual simplex method terminates and objective function \( 4x_1 - 2x_2 - x_3 \) is maximized with \(-\frac{17}{2}\) at \((0, 4, \frac{1}{2})\).
11.6 The Primal-Dual Algorithm

Let \((P2)\) be a linear program in standard form

\[
\begin{align*}
\text{maximize} & \quad cx \\
\text{subject to} & \quad Ax = b \text{ and } x \geq 0,
\end{align*}
\]

where \(A\) is an \(m \times n\) matrix of rank \(m\), and \((D)\) be its dual given by

\[
\begin{align*}
\text{minimize} & \quad yb \\
\text{subject to} & \quad yA \geq c,
\end{align*}
\]

where \(y \in (R^m)^*\).

First, we may assume that \(b \geq 0\) by changing every equation \(\sum_{j=1}^n a_{ij}x_j = b_i\) with \(b_i < 0\) to \(\sum_{j=1}^n -a_{ij}x_j = -b_i\). If we happen to have some feasible solution \(y\) of the dual program \((D)\), we know from Theorem 28.12 that a feasible solution \(x\) of \((P2)\) is an optimal solution iff the equations in \((*)_P\) hold. If we denote by \(J\) the subset of \(\{1, \ldots, n\}\) for which the equalities

\[yA^J = c_j\]

hold, then by Theorem 28.12 a feasible solution \(x\) of \((P2)\) is an optimal solution iff

\[x_j = 0 \quad \text{for all } j \notin J.\]

Let \(|J| = p\) and \(N = \{1, \ldots, n\} - J\). The above suggests looking for \(x \in R^n\) such that

\[
\sum_{j \in J} x_j A^j = b
\]

\[
x_j \geq 0 \quad \text{for all } j \in J
\]

\[
x_j = 0 \quad \text{for all } j \notin J,
\]

or equivalently

\[
A_J x_J = b, \quad x_J \geq 0, \quad (*)_1
\]

and

\[
x_N = 0_{n-p}.
\]

To search for such an \(x\), and just need to look for a feasible \(x_J\), and for this we can use the restricted primal linear program \((RP)\) defined as follows:

\[
\begin{align*}
\text{maximize} & \quad - (\xi_1 + \cdots + \xi_m) \\
\text{subject to} & \quad (A_J, I_m) \begin{pmatrix} x_J \\ \xi \end{pmatrix} = b \text{ and } x, \xi \geq 0.
\end{align*}
\]
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Since by hypothesis $b \geq 0$ and the objective function is bounded above by 0, this linear program has an optimal solution $(x^*_J, \xi^*)$.

If $\xi^* = 0$, then the vector $u^* \in \mathbb{R}^n$ given by $u^*_J = x^*_J$ and $u^*_N = 0_{n-p}$ is an optimal solution of $(P)$.

Otherwise, $\xi^* > 0$ and we have failed to solve $(*)_1$. However we may try to use $\xi^*$ to improve $y$. For this, consider the dual $(DRP)$ of $(RP)$:

$$\begin{array}{rcl}
\text{minimize} & zb \\
\text{subject to} & zA_J \geq 0 \\
& z \geq -1_m^T.
\end{array}$$

Observe that the program $(DRP)$ has the same objective function as the original dual program $(D)$. We know by Theorem 28.11 that the optimal solution $(x^*_J, \xi^*)$ of $(RP)$ yields an optimal solution $z^*$ of $(DRP)$ such that

$$z^*b = -(\xi^*_1 + \cdots + \xi^*_m) < 0.$$ 

In fact, if $K^*$ is the basis associated with $(x^*_J, \xi^*)$ and if we write

$$\tilde{A} = (A_J \quad I_m)$$

and $\tilde{c} = [0_p^T \quad -1_m^T]$, then by Theorem 28.11 we have

$$z^* = \tilde{c}_{K^*} \tilde{A}_{K^*}^{-1} = -1_m^T - (\tilde{c}_{K^*})_{(p+1, \ldots, p+m)},$$

where $(\tilde{c}_{K^*})_{(p+1, \ldots, p+m)}$ denotes the row vector of reduced costs in the final tableau corresponding to the last $m$ columns.

If we write

$$y(\theta) = y + \theta z^*,$$

then the new value of the objective function of $(D)$ is

$$y(\theta)b = yb + \theta z^*b,$$

and since $z^*b < 0$, we have a chance of improving the objective function of $(D)$, that is, decreasing its value for $\theta > 0$ small enough if $y(\theta)$ is feasible for $(D)$. This will be the case iff $y(\theta)A \geq c$ iff

$$yA + \theta z^*A \geq c.$$  

(*3)

Now since $y$ is a feasible solution of $(D)$ we have $yA \geq c$, so if $z^*A \geq 0$ then $(*)_3$ is satisfied and $y(\theta)$ is a solution of $(D)$ for all $\theta > 0$, which means that $(D)$ is unbounded. But this implies that $(P)$ is not feasible.

Let us take a closer look at the inequalities $z^*A \geq 0$. For $j \in J$, Since $z^*$ is an optimal solution of $(DRP)$, we know that $z^*A_J \geq 0$, so if $z^*A^*_J \geq 0$ for all $j \in N$, then $(P)$ is not feasible.
11.6. THE PRIMAL-DUAL ALGORITHM

Otherwise, there is some $j \in N = \{1, \ldots, n\} - J$ such that

$$z^* A^j < 0,$$

and then since by the definition of $J$ we have $y A^j > c_j$ for all $j \in N$, if we pick $\theta > 0$ such that

$$\theta \leq \frac{y A^j - c_j}{-z^* A^j} \quad j \in N, \ z^* A^j < 0,$$

then we decrease the objective function $y(\theta)b = yb + \theta z^*b$ of $(D)$ (since $z^*b < 0$). Therefore we pick the best $\theta$, namely

$$\theta^+ = \min \left\{ \frac{y A^j - c_j}{-z^* A^j} \left| j \notin J, \ z^* A^j < 0 \right\} > 0. \quad (\ast_4)$$

Next, we update $y$ to $y^+ = y(\theta^+) = y + \theta^+ z^*$, we create the new restricted primal with the new subset

$$J^+ = \{ j \in \{1, \ldots, n\} | y^+ A^j = c_j \},$$

and repeat the process. Here are the steps of the primal-dual algorithm.

Step 1. Find some feasible solution $y$ of the dual program $(D)$. We will show later that this is always possible.

Step 2. Compute

$$J^+ = \{ j \in \{1, \ldots, n\} | y^+ A^j = c_j \}.$$

Step 3. Set $J = J^+$ and solve the problem $(RP)$ using the simplex algorithm, starting from the optimal solution determined during the previous round, obtaining the optimal solution $(x^*_J, \xi^*)$ with the basis $K^*$.

Step 4.

If $\xi^* = 0$, then stop with an optimal solution $u^*$ for $(P)$ such that $u^*_J = x^*_J$ and the other components of $u^*$ are zero.

Else let

$$z^* = -1^*_m - (c_{K^*})_{(p+1, \ldots, p+m)},$$

be the optimal solution of $(DRP)$ corresponding to $(x^*_J, \xi^*)$ and the basis $K^*$.

If $z^* A^j \geq 0$ for all $j \notin J$, then stop; the program $(P)$ has no feasible solution.

Else compute

$$\theta^+ = \min \left\{ \frac{y A^j - c_j}{z^* A^j} \left| j \notin J, \ z^* A^j < 0 \right\}, \quad y^+ = y + \theta^+ z^*,$$

and

$$J^+ = \{ j \in \{1, \ldots, n\} | y^+ A^j = c_j \}.$$

Go back to Step 3.

The following proposition shows that at each iteration we can start the program $(RP)$ with the optimal solution obtained at the previous iteration.
**Proposition 11.13.** Every $j \in J$ such that $A^j$ is in the basis of the optimal solution $\xi^*$ belongs to the next index set $J^+$.

**Proof.** Such an index $j \in J$ correspond to a variable $\xi_j$ such that $\xi_j > 0$, so by complementary slackness, the constraint $z^* A^j \geq 0$ of the dual program ($DRP$) must be an equality, that is, $z^* A^j = 0$. But then, we have

$$y^+ A^j = y A^j + \theta^+ z^* A^j = c_j,$$

which shows that $j \in J^+$. \qed

If $(u^*, \xi^*)$ with the basis $K^*$ is the optimal solution of the program $(RP)$, Proposition 28.13 together with the last property of Theorem 28.11 allows us to restart the $(RP)$ in Step 3 with $(u^*, \xi^*)_{K^*}$ as initial solution (with basis $K^*$). For every $j \in J - J^+$, column $j$ is deleted, and for every $j \in J^+ - J$, the new column $A^j$ is computed by multiplying $\hat{A}_{K^*}^{-1}$ and $A^j$, but $\hat{A}_{K^*}^{-1}$ is the matrix $\Gamma^* [1:m; p+1:p+m]$ consisting of the last $m$ columns of $\Gamma^*$ in the final tableau, and the new reduced $\tilde{c}_j$ is given by $c_j - z^* A^j$. Reusing the optimal solution of the previous $(RP)$ may improve efficiency significantly.

Another crucial observation is that for any index $j_0 \in N$ such that

$$\theta^+ = (y A^{j_0} - c_{j_0}) / (-z^* A^{j_0}),$$

we have

$$y^+ A_{j_0} = y A^{j_0} + \theta^+ z^* A^{j_0} = c_{j_0},$$

and so $j_0 \in J^+$. This fact that be used to ensure that the primal-dual algorithm terminates in a finite number of steps (using a pivot rule that prevents cycling); see Papadimitriou and Steiglitz [80] (Theorem 5.4).

It remains to discuss how to pick some initial feasible solution $y$ of the dual program $(D)$. If $c_j \leq 0$ for $j = 1, \ldots, n$, then we can pick $y = 0$.

We should note that in many applications, the natural primal optimization problem is actually the *minimization* some objective function $cx = c_1 x_1 + \cdots + c_n x_n$, rather its maximization. For example, many of the optimization problems considered in Papadimitriou and Steiglitz [80] are minimization problems.

Of course, minimizing $cx$ is equivalent to maximizing $-cx$, so our presentation covers minimization too. But if we are dealing with a minimization problem, the weight $c_j$ are often nonnegative, so from the point of view of maximization we will have $-c_j \leq 0$ for all $j$, and we will be able to use $y = 0$ as a starting point.

Going back to our primal problem in maximization form and its dual in minimization form, we still need to deal with the situation where $c_j > 0$ for some $j$, in which case there may not be any obvious $y$ feasible for $(D)$. Preferably we would like to find such a $y$ very cheaply.
There is a trick to deal with this situation. We pick some very large positive number $M$ and add to the set of equations $Ax = b$ the new equation

$$x_1 + \cdots + x_n + x_{n+1} = M,$$

with the new variable $x_{n+1}$ constrained to be nonnegative. If the program $(P)$ has a feasible solution, such an $M$ exists. In fact, it can shown that for any basic feasible solution $u = (u_1, \ldots, u_n)$, each $|u_i|$ is bounded by some expression depending only on $A$ and $b$; see Papadimitriou and Steiglitz [80] (Lemma 2.1). The proof is not difficult and relies on the fact that the inverse of a matrix can be expressed in terms of certain determinants (the adjugates). Unfortunately, this bound contains $m!$ as a factor, which makes it quite impractical.

Having added the new equation above, we obtain the new set of equations

$$\begin{pmatrix} A & 0_n \\ 1_n^T & 1 \end{pmatrix} \begin{pmatrix} x \\ x_{n+1} \end{pmatrix} = \begin{pmatrix} b \\ M \end{pmatrix},$$

with $x \geq 0, x_{n+1} \geq 0$, and the new objective function given by

$$\begin{pmatrix} c & 0 \end{pmatrix} \begin{pmatrix} x \\ x_{n+1} \end{pmatrix} = cx.$$

The dual of the above linear program is

$$\begin{align*}
\text{minimize} & \quad y b + y_{m+1} M \\
\text{subject to} & \quad y A^j + y_{m+1} \geq c_j \quad j = 1, \ldots, n \\
& \quad y_{m+1} \geq 0.
\end{align*}$$

If $c_j > 0$ for some $j$, observe that the linear form $\tilde{y}$ given by

$$\tilde{y}_i = \begin{cases} 0 & \text{if } 1 \leq i \leq m \\
\max_{1 \leq j \leq n} \{c_j\} & > 0 \end{cases}$$

is a feasible solution of the new dual program. In practice, we can choose $M$ to be a number close to the largest integer representable on the computer being used.

Here is an example of the primal-dual algorithm given in the Math 588 class notes of T. Molla.

**Example 11.3.** Consider the following linear program in standard form:

Maximize $-x_1 - 3x_2 - 3x_3 - x_4$

subject to

$$\begin{pmatrix} 3 & 4 & -3 & 1 \\ 3 & -2 & 6 & -1 \\ 6 & 4 & 0 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \begin{pmatrix} 2 \\ 1 \\ 4 \end{pmatrix}$$

and $x_1, x_2, x_3, x_4 \geq 0$. 
The associated dual program \((D)\) is

\[
\text{Minimize } 2y_1 + y_2 + 4y_3 \\
\text{subject to } \begin{pmatrix} y_1 & y_2 & y_3 \end{pmatrix} \begin{pmatrix} 3 & 4 & -3 & 1 \\ 3 & -2 & 6 & -1 \\ 6 & 4 & 0 & 1 \end{pmatrix} \geq \begin{pmatrix} -1 \\ -3 \\ -3 \\ -1 \end{pmatrix}.
\]

We initialize the primal-dual algorithm with the dual feasible point \(y = (-1/3, 0, 0)\). Observe that only the first inequality of \((D)\) is actually an equality, and hence \(J = \{1\}\). We form the restricted primal program \((RP1)\)

\[
\text{Maximize } - (\xi_1 + \xi_2 + \xi_3) \\
\text{subject to } \begin{pmatrix} 3 & 1 & 0 & 0 \\ 3 & 0 & 1 & 0 \\ 6 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ \xi_1 \\ \xi_2 \\ \xi_3 \end{pmatrix} = \begin{pmatrix} 2 \\ 1 \\ 4 \end{pmatrix} \text{ and } x_1, \xi_1, \xi_2, \xi_3 \geq 0.
\]

We now solve \((RP1)\) via the simplex algorithm. The initial tableau with \(K = (2, 3, 4)\) and \(J = \{1\}\) is

\[
\begin{array}{cccc|c}
 & x_1 & \xi_1 & \xi_2 & \xi_3 \\
7 & 12 & 0 & 0 & 0 \\
\xi_1 = 2 & 3 & 1 & 0 & 0 \\
\xi_2 = 1 & 0 & 1 & 0 \\
\xi_3 = 4 & 6 & 0 & 0 & 1 \\
\end{array}
\]

For \((RP1)\), \(c = (0, -1, -1, -1)\), \((x_1, \xi_1, \xi_2, \xi_3) = (0, 2, 1, 4)\), and the nonzero reduced cost is given by

\[
0 - (-1 - 1 - 1) \begin{pmatrix} 3 \\ 3 \\ 6 \end{pmatrix} = 12.
\]

Since there is only one nonzero reduced cost, we must set \(j^+ = 1\). Since \(\min\{\xi_1/3, \xi_2/3, \xi_3/6\} = 1/3\), we see that \(k^- = 3\) and \(K = (2, 1, 4)\). Hence we pivot through the red circled 3 (namely we divide row 2 by 3, and then subtract \(3 \times (\text{row 2})\) from row 1, \(6 \times (\text{row 2})\) from row 3, and \(12 \times (\text{row 2})\) from row 0), to obtain the tableau

\[
\begin{array}{cccc|c}
 & x_1 & \xi_1 & \xi_2 & \xi_3 \\
3 & 0 & 0 & -4 & 0 \\
\xi_1 = 1 & 0 & 1 & -1 & 0 \\
x_1 = 1/3 & 1 & 0 & 1/3 & 0 \\
\xi_3 = 2 & 0 & 0 & -2 & 1 \\
\end{array}
\]

At this stage the simplex algorithm for \((RP1)\) terminates since there are no positive reduced costs. Since the upper left corner of the final tableau is not zero, we proceed with Step 4 of
the primal dual algorithm and compute
\[ z^* = (-1 - 1 - 1) - (0 - 4 0) = (-1 3 - 1), \]
\[ (-1/3 0 0) \begin{pmatrix} 4 \\ -2 \\ 4 \end{pmatrix} + 3 = \frac{5}{3}, \quad -(-1 3 - 1) \begin{pmatrix} 4 \\ -2 \\ 4 \end{pmatrix} = 14, \]
\[ (-1/3 0 0) \begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix} + 1 = \frac{2}{3}, \quad -(-1 3 - 1) \begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix} = 5, \]
so
\[ \theta^+ = \min \left\{ \frac{5}{42}, \frac{2}{15} \right\} = \frac{5}{42}, \]
and we conclude that the new feasible solution for \((D)\) is
\[ y^+ = (-1/3 0 0) + \frac{5}{42}(-1 3 - 1) = (-19/42 5/14 - 5/42). \]

When we substitute \(y^+\) into \((D)\), we discover that the first two constraints are equalities, and that the new \(J\) is \(J = \{1, 2\}\). The new reduced primal \((RP2)\) is

Maximize \(- (\xi_1 + \xi_2 + \xi_3)\)

subject to
\[ \begin{pmatrix} 3 & 4 & 1 & 0 & 0 \\ 3 & -2 & 0 & 1 & 0 \\ 6 & 4 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \xi_1 \\ \xi_2 \\ \xi_3 \end{pmatrix} = \begin{pmatrix} 2 \\ 1 \\ 4 \end{pmatrix} \]
and \(x_1, x_2, \xi_1, \xi_2, \xi_3 \geq 0\).

Once again, we solve \((RP2)\) via the simplex algorithm, where \(c = (0, 0, -1, -1, -1)\), \((x_1, x_2, \xi_1, \xi_2, \xi_3) = (1/3, 0, 1, 0, 2)\) and \(K = (3, 1, 5)\). The initial tableau is obtained from the final tableau of the previous \((RP1)\) by adding a column corresponding to the variable \(x_2\), namely
\[ \hat{A}^{-1}_K A^2 = \begin{pmatrix} 1 & -1 & 0 \\ 0 & 1/3 & 0 \\ 0 & -2 & 1 \end{pmatrix} \begin{pmatrix} 4 \\ -2 \\ 4 \end{pmatrix} = \begin{pmatrix} 6 \\ -2/3 \\ -1 \end{pmatrix}, \]
with
\[ \bar{c}_2 = c_2 - z^* A^2 = 0 - (-1 3 - 1) \begin{pmatrix} 4 \\ -2 \\ 4 \end{pmatrix} = 14, \]
and we get

<table>
<thead>
<tr>
<th></th>
<th>(x_1)</th>
<th>(x_2)</th>
<th>(\xi_1)</th>
<th>(\xi_2)</th>
<th>(\xi_3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(x_1 = 1/3)</td>
<td>1</td>
<td>-2/3</td>
<td>0</td>
<td>1/3</td>
<td>0</td>
</tr>
<tr>
<td>(\xi_3 = 2)</td>
<td>0</td>
<td>8</td>
<td>0</td>
<td>-2</td>
<td>1</td>
</tr>
<tr>
<td>(\xi_1 = 1)</td>
<td>0</td>
<td>6</td>
<td>1</td>
<td>-1</td>
<td>0</td>
</tr>
</tbody>
</table>
Note that \( j^+ = 2 \) since the only positive reduced cost occurs in column 2. Also observe that since \( \min\{\xi_1/6, \xi_3/8\} = \xi_1/6 = 1/6 \), we set \( k^- = 3 \), \( K = (2, 1, 5) \) and pivot along the red 6 to obtain the tableau

\[
\begin{array}{c|cccc}
  & x_1 & x_2 & \xi_1 & \xi_2 \\
\hline
2/3 & 0 & 0 & -7/3 & -5/3 \\
x_2 = 1/6 & 0 & 1 & 1/6 & -1/6 \\
x_1 = 4/9 & 1 & 0 & 1/9 & 2/9 \\
\xi_3 = 2/3 & 0 & 0 & -4/3 & -2/3 \\
\end{array}
\]

Since the reduced costs are either zero or negative the simplex algorithm terminates, and we compute

\[
z^* = (-1 - 1 - 1) - (-7/3 - 5/3 0) = (4/3 2/3 - 1),
\]

\[
(-19/42 5/14 - 5/42) \begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix} + 1 = 1/14, \quad -(4/3 2/3 - 1) \begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix} = 1/3,
\]

so

\[
\theta^+ = \frac{3}{14},
\]

\[
y^+ = (-19/42 5/14 - 5/42) + \frac{5}{14} (4/3 2/3 - 1) = (-1/6 1/2 - 1/3).
\]

When we plug \( y^+ \) into \((D)\), we discover that the first, second, and fourth constraints are equalities, which implies \( J = \{1, 2, 4\} \). Hence the new restricted primal \((RP3)\) is

Maximize \(- (\xi_1 + \xi_2 + \xi_3)\)

subject to

\[
\begin{pmatrix}
  3 & 4 & 1 & 1 & 0 & 0 \\
  3 & -2 & -1 & 0 & 1 & 0 \\
  6 & 4 & 1 & 0 & 0 & 1 \\
\end{pmatrix}
\begin{pmatrix}
  x_1 \\
  x_2 \\
  x_4 \\
  \xi_1 \\
  \xi_2 \\
  \xi_3 \\
\end{pmatrix}

= \begin{pmatrix}
  2 \\
  1 \\
  4 \\
\end{pmatrix}
\text{ and } x_1, x_2, x_4, \xi_1, \xi_2, \xi_3 \geq 0.
\]

The initial tableau for \((RP3)\), with \( c = (0, 0, 0, -1, -1, -1) \), \( (x_1, x_2, x_4, \xi_1, \xi_2, \xi_3) = (4/9, 1/6, 0, 0, 0, 2/3) \) and \( K = (2, 1, 6) \), is obtained from the final tableau of the previous \((RP2)\) by adding a column corresponding the the variable \( x_4 \), namely

\[
\widehat{A}_K^{-1} A^4 = \begin{pmatrix}
  1/6 & -1/6 & 0 \\
  1/9 & 2/9 & 0 \\
  -4/3 & -2/3 & 1 \\
\end{pmatrix}
\begin{pmatrix}
  1 \\
  -1 \\
  1 \\
\end{pmatrix}

= \begin{pmatrix}
  1/3 \\
  -1/9 \\
  1/3 \\
\end{pmatrix},
\]

with

\[
\bar{c}_4 = c_4 - z^* A^4 = 0 - (4/3 2/3 - 1) \begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix} = 1/3,
\]
and we get

\[
\begin{array}{cccccc}
2/3 & 0 & 0 & 1/3 & -7/3 & -5/3 \\
0 & 0 & 1/3 & 1/6 & -1/6 & 0 \\
1/6 & 0 & 1 & (1/3) & 1/6 & -1/6 \\
4/9 & 1 & 0 & -1/9 & 1/9 & 2/9 \\
2/3 & 0 & 0 & 1/3 & -4/3 & -2/3 \\
\end{array}
\]

Since the only positive reduced cost occurs in column 3, we set \( j^+ = 3 \). Furthermore, since \( \min \{ x_2/(1/3), \xi_3/(1/3) \} = x_2/(1/3) = 1/2 \), we let \( k^- = 2 \), \( K = (3, 1, 6) \), and pivot around the red circled 1/3 to obtain

\[
\begin{array}{cccccc}
1/2 & 0 & -1 & 0 & -5/2 & -3/2 \\
0 & 3 & 1 & 1/2 & -1/2 & 0 \\
1 & 1/3 & 0 & 1/6 & 1/6 & 0 \\
0 & -1 & 0 & -3/2 & -1/2 & 1 \\
\end{array}
\]

At this stage, there are no positive reduced costs, and we must compute

\[
z^* = (-1 - 1 - 1) - (-5/2 - 3/2 0) = (3/2 1/2 - 1),
\]

\[
(\begin{array}{ccc}
-1/6 & 1/2 & -1/3 \\
\end{array}) \begin{pmatrix}
-3 \\
6 \\
0
\end{pmatrix} + 3 = 13/2, \quad - (\begin{array}{ccc}
3/2 & 1/2 & -1 \\
\end{array}) \begin{pmatrix}
-3 \\
6 \\
0
\end{pmatrix} = 3/2,
\]

so

\[
\theta^+ = \frac{13}{3},
\]

\[
y^+ = (-1/6 1/2 - 1/3) + \frac{13}{3}(3/2 1/2 - 1) = (19/3 8/3 - 14/3).
\]

We plug \( y^+ \) into \((D)\) and discover that the first, third, and fourth constraints are equalities. Thus, \( J = \{1, 3, 4\} \) and the restricted primal \((RP4)\) is

\[
\begin{align*}
\text{Maximize} & \quad - (\xi_1 + \xi_2 + \xi_3) \\
\text{subject to} & \quad \begin{pmatrix}
3 & -3 & 1 & 0 & 0 \\
3 & 6 & -1 & 0 & 1 \\
6 & 0 & 1 & 0 & 0 \end{pmatrix} \begin{pmatrix}
x_1 \\
x_3 \\
x_4 \\
\xi_1 \\
\xi_2 \\
\xi_3
\end{pmatrix} = \begin{pmatrix}
2 \\
1 \\
4
\end{pmatrix} \quad \text{and} \quad x_1, x_3, x_4, \xi_1, \xi_2, \xi_3 \geq 0.
\end{align*}
\]
The initial tableau for \((RP4)\), with \(c = (0, 0, 0, -1, -1)\), \((x_1, x_3, x_4, \xi_1, \xi_2, \xi_3) = (1/2, 0, 1/2, 0, 0, 1/2)\) and \(K = (3, 1, 6)\) is obtained from the final tableau of the previous \((RP3)\) by replacing the column corresponding to the variable \(x_2\) by a column corresponding to the variable \(x_3\), namely

\[
\hat{A}_K^{-1}A^3 = \begin{pmatrix}
0.5 & -0.5 & 0.5 & 0 & 0 & 0.5 \\
0.5 & -0.5 & 0 & 0.5 & 0 & 0.5 \\
-0.5 & 0.5 & 0 & 0 & 0.5 & 0.5
\end{pmatrix}
\begin{pmatrix}
-3 \\
6 \\
0
\end{pmatrix} = \begin{pmatrix}
-0.5 \\
0.5 \\
0
\end{pmatrix},
\]

with

\[
\bar{c}_3 = c_3 - z^*A^3 = 0 - (3/2 \ 1/2 \ -1) \begin{pmatrix}
-3 \\
6 \\
0
\end{pmatrix} = 3/2,
\]

and we get

\[
\begin{array}{ccccccc}
1/2 & x_1 & x_3 & x_4 & \xi_1 & \xi_2 & \xi_3 \\
0 & 3/2 & 0 & -5/2 & -3/2 & 0 \\
x_4 = 1/2 & 0 & -9/2 & 1 & 1/2 & -1/2 & 0 \\
x_1 = 1/2 & 1 & 1/2 & 0 & 1/6 & 1/6 & 0 \\
\xi_3 = 1/2 & 0 & 3/2 & 0 & -3/2 & -1/2 & 1
\end{array}
\]

By analyzing the top row of reduced cost, we see that \(j^+ = 2\). Furthermore, since \(\min\{x_1/(1/2), \xi_3/(3/2)\} = \xi_3/(3/2) = 1/3\), we let \(k^- = 6\), \(K = (3, 1, 2)\), and pivot along the red circled 3/2 to obtain

\[
\begin{array}{ccccccc}
0 & x_1 & x_3 & x_4 & \xi_1 & \xi_2 & \xi_3 \\
0 & 0 & 0 & 0 & -1 & -1 & -1 \\
x_4 = 2 & 0 & 0 & 1 & -4 & -2 & 3 \\
x_1 = 1/3 & 1 & 0 & 0 & 2/3 & 1/3 & -1/3 \\
x_3 = 1/3 & 0 & 1 & 0 & -1 & -1/3 & 2/3
\end{array}
\]

Since the upper left corner of the final tableau is zero and the reduced costs are all \(\leq 0\), we are finally finished. Then \(y = (19/3 \ 8/3 \ -14/3)\) is an optimal solution of \((D)\), but more importantly \((x_1, x_2, x_3, x_4) = (1/3, 0, 1/3, 2)\) is an optimal solution for our original linear program and provides an optimal value of \(-10/3\).

The primal-dual algorithm for linear programming doesn’t seem to be the favorite method to solve linear programs nowadays. But it is important because its basic principle, to use a restricted (simpler) primal problem involving an objective function with fixed weights, namely 1, and the dual problem to provide feedback to the primal by improving the objective function of the dual, has led to a whole class of combinatorial algorithms (often approximation algorithms) based on the primal-dual paradigm. The reader will get a taste of this kind of algorithm by consulting Papadimitriou and Steiglitz [80], where it is explained.
how classical algorithms such as Dijkstra’s algorithm for the shortest path problem, and Ford and Fulkerson’s algorithm for max flow can be derived from the primal-dual paradigm.
CHAPTER 11. LINEAR PROGRAMMING AND DUALITY
Part III

NonLinear Optimization
Chapter 12
Basics of Hilbert Spaces

Most of the “deep” results about the existence of minima of real-valued functions proven in Chapter 30 rely on two fundamental results of Hilbert space theory:

1. The projection lemma, which is a result about nonempty, closed, convex subsets of a Hilbert space $V$.

2. The Riesz representation theorem, which allows us to express a continuous linear form on a Hilbert space $V$ in terms of a vector in $V$ and the inner product on $V$.

The correctness of the Karush–Kuhn–Tucker conditions appearing in Lagrangian duality follows from a version of the Farkas–Minkowski proposition, which also follows from the projection lemma.

Thus we feel that it is indispensible to review some basic results of Hilbert space theory, although in most applications considered here the Hilbert space in question will be finite-dimensional. However, in optimization theory, there are many problems where we seek to find a function minimizing some type of energy functional (often given by a bilinear form), in which case we are dealing with an infinite dimensional Hilbert space, so it necessary to develop tools to deal with the more general situation of infinite-dimensional Hilbert spaces.

12.1 The Projection Lemma, Duality

Given a Hermitian space $(E, \varphi)$, we showed in Section 12.1 (Vol. I) that the function $\| \| : E \to \mathbb{R}$ defined such that $\| u \| = \sqrt{\varphi(u, u)}$, is a norm on $E$. Thus, $E$ is a normed vector space. If $E$ is also complete, then it is a very interesting space.

Recall that completeness has to do with the convergence of Cauchy sequences. A normed vector space $(E, \| \|)$ is automatically a metric space under the metric $d$ defined such that $d(u, v) = \| v - u \|$ (see Chapter 19 for the definition of a normed vector space and of a metric space, or Lang [65, 66], or Dixmier [35]). Given a metric space $E$ with metric $d$, a sequence
(a_n)_{n \geq 1} of elements a_n \in E is a Cauchy sequence iff for every \( \epsilon > 0 \), there is some \( N \geq 1 \) such that
\[ d(a_m, a_n) < \epsilon \quad \text{for all} \quad m, n \geq N. \]
We say that \( E \) is complete iff every Cauchy sequence converges to a limit (which is unique, since a metric space is Hausdorff).

Every finite dimensional vector space over \( \mathbb{R} \) or \( \mathbb{C} \) is complete. For example, one can show by induction that given any basis \( (e_1, \ldots, e_n) \) of \( E \), the linear map \( h: \mathbb{C}^n \to E \) defined such that
\[ h((z_1, \ldots, z_n)) = z_1e_1 + \cdots + z_ne_n \]
is a homeomorphism (using the sup-norm on \( \mathbb{C}^n \)). One can also use the fact that any two norms on a finite dimensional vector space over \( \mathbb{R} \) or \( \mathbb{C} \) are equivalent (see Chapter 7 (Vol. I), or Lang [66], Dixmier [35], Schwartz [91]).

However, if \( E \) has infinite dimension, it may not be complete. When a Hermitian space is complete, a number of the properties that hold for finite dimensional Hermitian spaces also hold for infinite dimensional spaces. For example, any closed subspace has an orthogonal complement, and in particular, a finite dimensional subspace has an orthogonal complement. Hermitian spaces that are also complete play an important role in analysis. Since they were first studied by Hilbert, they are called Hilbert spaces.

**Definition 12.1.** A (complex) Hermitian space \( \langle E, \varphi \rangle \) which is a complete normed vector space under the norm \( \| \| \) induced by \( \varphi \) is called a Hilbert space. A real Euclidean space \( \langle E, \varphi \rangle \) which is complete under the norm \( \| \| \) induced by \( \varphi \) is called a real Hilbert space.

All the results in this section hold for complex Hilbert spaces as well as for real Hilbert spaces. We state all results for the complex case only, since they also apply to the real case, and since the proofs in the complex case need a little more care.

**Example 12.1.** The space \( l^2 \) of all countably infinite sequences \( x = (x_i)_{i \in \mathbb{N}} \) of complex numbers such that \( \sum_{i=0}^{\infty} |x_i|^2 < \infty \) is a Hilbert space. It will be shown later that the map \( \varphi: l^2 \times l^2 \to \mathbb{C} \) defined such that
\[ \varphi((x_i)_{i \in \mathbb{N}}, (y_i)_{i \in \mathbb{N}}) = \sum_{i=0}^{\infty} x_i\overline{y_i} \]
is well defined, and that \( l^2 \) is a Hilbert space under \( \varphi \). In fact, we will prove a more general result (Proposition A.3).

**Example 12.2.** The set \( C^\infty[a, b] \) of smooth functions \( f: [a, b] \to \mathbb{C} \) is a Hermitian space under the Hermitian form
\[ \langle f, g \rangle = \int_a^b f(x)\overline{g(x)}dx, \]
but it is not a Hilbert space because it is not complete. It is possible to construct its completion \( L^2([a, b]) \), which turns out to be the space of Lebesgue integrable functions on \([a, b]\).
Theorem 19.22 yields a quick proof of the fact that any Hermitian space $E$ (with Hermitian product $\langle -, - \rangle$) can be embedded in a Hilbert space $E_h$.

**Theorem 12.1.** Given a Hermitian space $(E, \langle -, - \rangle)$ (resp. Euclidean space), there is a Hilbert space $(E_h, \langle -, - \rangle_h)$ and a linear map $\varphi: E \to E_h$, such that

$$\langle u, v \rangle = \langle \varphi(u), \varphi(v) \rangle_h$$

for all $u, v \in E$, and $\varphi(E)$ is dense in $E_h$. Furthermore, $E_h$ is unique up to isomorphism.

**Proof.** Let $(\hat{E}, \|\|_{\hat{E}})$ be the Banach space, and let $\varphi: E \to \hat{E}$ be the linear isometry, given by Theorem 19.22. Let $\|u\| = \sqrt{\langle u, u \rangle}$ and $E_h = \hat{E}$. If $E$ is a real vector space, we know from Section 10.1 (Vol. I) that the inner product $\langle -, - \rangle$ can be expressed in terms of the norm $\|u\|$ by the polarity equation

$$\langle u, v \rangle = \frac{1}{2}(\|u + v\|^2 - \|u\|^2 - \|v\|^2),$$

and if $E$ is a complex vector space, we know from Section 12.1 (Vol. I) that we have the polarity equation

$$\langle u, v \rangle = \frac{1}{4}(\|u + v\|^2 - \|u - v\|^2 + i\|u + iv\|^2 - i\|u - iv\|^2).$$

By the Cauchy-Schwarz inequality, $|\langle u, v \rangle| \leq \|u\|\|v\|$, the map $\langle -, - \rangle: E \times E \to \mathbb{C}$ (resp. $\langle -, - \rangle: E \times E \to \mathbb{R}$) is continuous. However, it is not uniformly continuous, but we can get around this problem by using the polarity equations to extend it to a continuous map. By continuity, the polarity equations also hold in $E_h$, which shows that $\langle -, - \rangle$ extends to a positive definite Hermitian inner product (resp. Euclidean inner product) $\langle -, - \rangle_h$ on $E_h$ induced by $\|\|_{\hat{E}}$, extending $\langle -, - \rangle$.

**Proof.** We followed the approach in Schwartz [90] (Chapter XXIII, Section 42. Theorem 2). For other approaches, see Munkres [78] (Chapter 7, Section 43), and Bourbaki [21].

One of the most important facts about finite-dimensional Hermitian (and Euclidean) spaces is that they have orthonormal bases. This implies that, up to isomorphism, every finite-dimensional Hermitian space is isomorphic to $\mathbb{C}^n$ (for some $n \in \mathbb{N}$) and that the inner product is given by

$$\langle (x_1, \ldots, x_n), (y_1, \ldots, y_n) \rangle = \sum_{i=1}^{n} x_i \overline{y_i}.$$ 

Furthermore, every subspace $W$ has an orthogonal complement $W^\perp$, and the inner product induces a natural duality between $E$ and $E^*$ (actually, between $\overline{E}$ and $E^*$) where $E^*$ is the space of linear forms on $E$.

When $E$ is a Hilbert space, $E$ may be infinite dimensional, often of uncountable dimension. Thus, we can’t expect that $E$ always have an orthonormal basis. However, if we modify
the notion of basis so that a “Hilbert basis” is an orthogonal family that is also dense in \( E \), i.e., every \( v \in E \) is the limit of a sequence of finite combinations of vectors from the Hilbert basis, then we can recover most of the “nice” properties of finite-dimensional Hermitian spaces. For instance, if \( (u_k)_{k \in K} \) is a Hilbert basis, for every \( v \in E \), we can define the Fourier coefficients \( c_k = \langle v, u_k \rangle / \| u_k \| \), and then, \( v \) is the “sum” of its Fourier series \( \sum_{k \in K} c_k u_k \). However, the cardinality of the index set \( K \) can be very large, and it is necessary to define what it means for a family of vectors indexed by \( K \) to be summable. We will do this in Section A.1. It turns out that every Hilbert space is isomorphic to a space of the form \( l^2(K) \), where \( l^2(K) \) is a generalization of the space of Example 29.1 (see Theorem A.8, usually called the Riesz-Fischer theorem).

Our first goal is to prove that a closed subspace of a Hilbert space has an orthogonal complement. We also show that duality holds if we redefine the dual \( E' \) of \( E \) to be the space of continuous linear maps on \( E \). Our presentation closely follows Bourbaki [21]. We also were inspired by Rudin [83], Lang [65, 66], Schwartz [91, 90], and Dixmier [35]. In fact, we highly recommend Dixmier [35] as a clear and simple text on the basics of topology and analysis. We first prove the so-called projection lemma.

Recall that in a metric space \( E \), a subset \( X \) of \( E \) is closed iff for every convergent sequence \( (x_n) \) of points \( x_n \in X \), the limit \( x = \lim_{n \to \infty} x_n \) also belongs to \( X \). The closure \( \overline{X} \) of \( X \) is the set of all limits of convergent sequences \( (x_n) \) of points \( x_n \in X \). Obviously, \( X \subseteq \overline{X} \). We say that the subset \( X \) of \( E \) is dense in \( E \) iff \( E = \overline{X} \), the closure of \( X \), which means that every \( a \in E \) is the limit of some sequence \( (x_n) \) of points \( x_n \in X \). Convex sets will again play a crucial role.

First, we state the following easy “parallelogram inequality”, whose proof is left as an exercise.

**Proposition 12.2.** If \( E \) is a Hermitian space, for any two vectors \( u, v \in E \), we have

\[
\|u + v\|^2 + \|u - v\|^2 = 2(\|u\|^2 + \|v\|^2).
\]

From the above, we get the following proposition:

**Proposition 12.3.** If \( E \) is a Hermitian space, given any \( d, \delta \in \mathbb{R} \) such that \( 0 \leq \delta < d \), let

\[
B = \{ u \in E \mid \|u\| < d \} \quad \text{and} \quad C = \{ u \in E \mid \|u\| \leq d + \delta \}.
\]

For any convex set such \( A \) that \( A \subseteq C - B \), we have

\[
\|v - u\| \leq \sqrt{12d\delta},
\]

for all \( u, v \in A \) (see Figure 29.1).
12.1. THE PROJECTION LEMMA, DUALITY

Proof. Since $A$ is convex, $\frac{1}{2}(u + v) \in A$ if $u, v \in A$, and thus, $\|\frac{1}{2}(u + v)\| \geq d$. From the parallelogram inequality written in the form

$$\|\frac{1}{2}(u + v)\|^2 + \|\frac{1}{2}(u - v)\|^2 = \frac{1}{2}(\|u\|^2 + \|v\|^2),$$

since $\delta < d$, we get

$$\|\frac{1}{2}(u - v)\|^2 = \frac{1}{2}(\|u\|^2 + \|v\|^2) - \|\frac{1}{2}(u + v)\|^2 \leq (d + \delta)^2 - d^2 = 2d\delta + \delta^2 \leq 3d\delta,$$

from which

$$\|v - u\| \leq \sqrt{12d\delta}.$$  

$\square$

If $X$ is a nonempty subset of a metric space $(E, d)$, for any $a \in E$, recall that we define the distance $d(a, X)$ of $a$ to $X$ as

$$d(a, X) = \inf_{b \in X} d(a, b).$$

Also, the diameter $\delta(X)$ of $X$ is defined by

$$\delta(X) = \sup\{d(a, b) \mid a, b \in X\}.$$  

It is possible that $\delta(X) = \infty$. We leave the following standard two facts as an exercise (see Dixmier [35]):

**Proposition 12.4.** Let $E$ be a metric space.

(1) For every subset $X \subseteq E$, $\delta(X) = \delta(\overline{X})$.

(2) If $E$ is a complete metric space, for every sequence $(F_n)$ of closed nonempty subsets of $E$ such that $F_{n+1} \subseteq F_n$, if $\lim_{n \to \infty} \delta(F_n) = 0$, then $\bigcap_{n=1}^{\infty} F_n$ consists of a single point.
We are now ready to prove the crucial projection lemma.

**Proposition 12.5.** *(Projection lemma)* Let $E$ be a Hilbert space.

1. For any nonempty convex and closed subset $X \subseteq E$, for any $u \in E$, there is a unique vector $p_X(u) \in X$ such that
   \[ ||u - p_X(u)|| = \inf_{v \in X} ||u - v|| = d(u, X). \]
   See Figure 29.2.

2. The vector $p_X(u)$ is the unique vector $w \in E$ satisfying the following property (see Figure 29.3):
   \[ w \in X \quad \text{and} \quad \Re \langle u - w, z - w \rangle \leq 0 \quad \text{for all } z \in X. \quad (\ast) \]

3. If $X$ is a nonempty closed subspace of $E$ then the vector $p_X(u)$ is the unique vector $w \in E$ satisfying the following property:
   \[ w \in X \quad \text{and} \quad \langle u - w, z \rangle = 0 \quad \text{for all } z \in X. \quad (\ast\ast) \]

![Figure 12.2: Let $X$ be the solid pink ellipsoid. The projection of the purple point $u$ onto $X$ is the magenta point $p_X(u)$.](image)

**Proof.** (1) Let $d = \inf_{v \in X} ||u - v|| = d(u, X)$. We define a sequence $X_n$ of subsets of $X$ as follows: for every $n \geq 1$,

\[ X_n = \left\{ v \in X \mid ||u - v|| \leq d + \frac{1}{n} \right\}. \]
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It is immediately verified that each $X_n$ is nonempty (by definition of $d$), convex, and that $X_{n+1} \subseteq X_n$. Also, by Proposition 29.3, we have

$$\sup\{\|w - v\| \mid v, w \in X_n\} \leq \sqrt{12d/n},$$

and thus, $\bigcap_{n \geq 1} X_n$ contains at most one point. We will prove that $\bigcap_{n \geq 1} X_n$ contains exactly one point, namely, $p_X(u)$. For this, define a sequence $(w_n)_{n \geq 1}$ by picking some $w_n \in X_n$ for every $n \geq 1$. We claim that $(w_n)_{n \geq 1}$ is a Cauchy sequence. Given any $\epsilon > 0$, if we pick $N$ such that

$$N > \frac{12d}{\epsilon^2},$$

since $(X_n)_{n \geq 1}$ is a monotonic decreasing sequence, which means that $X_{n+1} \subseteq X_n$ for all $n \geq 1$, for all $m, n \geq N$, we have

$$\|w_m - w_n\| \leq \sqrt{12d/N} < \epsilon,$$

as desired. Since $E$ is complete, the sequence $(w_n)_{n \geq 1}$ has a limit $w$, and since $w_n \in X$ and $X$ is closed, we must have $w \in X$. Also observe that

$$\|u - w\| \leq \|u - w_n\| + \|w_n - w\|,$$

and since $w$ is the limit of $(w_n)_{n \geq 1}$ and

$$\|u - w_n\| \leq d + \frac{1}{n},$$

given any $\epsilon > 0$, there is some $n$ large enough so that

$$\frac{1}{n} < \frac{\epsilon}{2} \quad \text{and} \quad \|w_n - w\| \leq \frac{\epsilon}{2},$$

and thus

$$\|u - w\| \leq d + \epsilon.$$
Since the above holds for every $\epsilon > 0$, we have $\|u - w\| = d$. Thus, $w \in X_n$ for all $n \geq 1$, which proves that $\bigcap_{n \geq 1} X_n = \{w\}$. Now, any $z \in X$ such that $\|u - z\| = d(u, X) = d$ also belongs to every $X_n$, and thus $z = w$, proving the uniqueness of $w$, which we denote as $p_X(u)$. See Figure 29.4.

Figure 12.4: Let $X$ be the solid pink ellipsoid with $p_X(u) = w$ at its apex. Each $X_n$ is the intersection of $X$ and a solid sphere centered at $u$ with radius $d + 1/n$. These intersections are the colored “caps” of Figure ii. The Cauchy sequence $(w_n)_{n \geq 1}$ is obtained by selecting a point in each colored $X_n$.

(2) Let $z \in X$. Since $X$ is convex, $w = (1 - \lambda)p_X(u) + \lambda z \in X$ for every $\lambda$, $0 \leq \lambda \leq 1$. Then, we have

$$\|u - w\| \geq \|u - p_X(u)\|$$

for all $\lambda$, $0 \leq \lambda \leq 1$, and since

$$\|u - w\|^2 = \|u - p_X(u) - \lambda(z - p_X(u))\|^2$$
$$= \|u - p_X(u)\|^2 + \lambda^2\|z - p_X(u)\|^2 - 2\lambda\Re\langle u - p_X(u), z - p_X(u) \rangle,$$

for all $\lambda$, $0 < \lambda \leq 1$, we get

$$\Re\langle u - p_X(u), z - p_X(u) \rangle = \frac{1}{2\lambda} \left(\|u - p_X(u)\|^2 - \|u - w\|^2\right) + \frac{\lambda}{2}\|z - p_X(u)\|^2,$$

and since this holds for every $\lambda$, $0 < \lambda \leq 1$ and

$$\|u - w\| \geq \|u - p_X(u)\|,$$

we have

$$\Re\langle u - p_X(u), z - p_X(u) \rangle \leq 0.$$
Conversely, assume that $w \in X$ satisfies the condition
\[ \Re \langle u - w, z - w \rangle \leq 0 \]
for all $z \in X$. For all $z \in X$, we have
\[ \| u - z \|^2 = \| u - w \|^2 + \| z - w \|^2 - 2 \Re \langle u - w, z - w \rangle \geq \| u - w \|^2, \]
which implies that $\| u - w \| = d(u, X) = d$, and from (1), that $w = p_X(u)$.

(3) If $X$ is a subspace of $E$ and $w \in X$, when $z$ ranges over $X$ the vector $z - w$ also ranges over the whole of $X$ so Condition (*) is equivalent to
\[ w \in X \quad \text{and} \quad \Re \langle u - w, z \rangle \leq 0 \quad \text{for all } z \in X. \]
Since $X$ is a subspace, if $z \in X$ then $-z \in X$, which implies that (*) is equivalent to
\[ w \in X \quad \text{and} \quad \Re \langle u - w, z \rangle = 0 \quad \text{for all } z \in X. \]
Finally, since $X$ is a subspace if $z \in X$ then $iz \in X$, and this implies that
\[ 0 = \Re \langle u - w, iz \rangle = -i \Im \langle u - w, z \rangle, \]
so $\Im \langle u - w, z \rangle = 0$, but since we also have $\Re \langle u - w, z \rangle = 0$, we see that (**) is equivalent to
\[ w \in X \quad \text{and} \quad \langle u - w, z \rangle = 0 \quad \text{for all } z \in X, \]
as claimed. \hfill \square

The vector $p_X(u)$ is called the projection of $u$ onto $X$, and the map $p_X : E \to X$ is called the projection of $E$ onto $X$. In the case of a real Hilbert space, there is an intuitive geometric interpretation of the condition
\[ \langle u - p_X(u), z - p_X(u) \rangle \leq 0 \]
for all $z \in X$. If we restate the condition as
\[ \langle u - p_X(u), p_X(u) - z \rangle \geq 0 \]
for all $z \in X$, this says that the absolute value of the measure of the angle between the vectors $u - p_X(u)$ and $p_X(u) - z$ is at most $\pi/2$. See Figure 29.5. This makes sense, since $X$ is convex, and points in $X$ must be on the side opposite to the “tangent space” to $X$ at $p_X(u)$, which is orthogonal to $u - p_X(u)$. Of course, this is only an intuitive description, since the notion of tangent space has not been defined!

If $X$ is a closed subspace of $E$, then Condition (**) says that the vector $u - p_X(u)$ is orthogonal to $X$, in the sense that $u - p_X(u)$ is orthogonal to every vector $z \in X$.

The map $p_X : E \to X$ is continuous, as shown below.
Figure 12.5: Let $X$ be the solid blue ice cream cone. The acute angle between the black vector $u - p_X(u)$ and the purple vector $p_X(u) - z$ is less than $\pi/2$.

**Proposition 12.6.** Let $E$ be a Hilbert space. For any nonempty convex and closed subset $X \subseteq E$, the map $p_X : E \to X$ is continuous. In fact, $p_X$ satisfies the Lipschitz condition

$$
\|p_X(v) - p_X(u)\| \leq \|v - u\| \quad \text{for all } u, v \in E.
$$

**Proof.** For any two vectors $u, v \in E$, let $x = p_X(u) - u$, $y = p_X(v) - p_X(u)$, and $z = v - p_X(v)$. Clearly, (as illustrated in Figure 29.6),

$$
v - u = x + y + z,
$$

and from Proposition 29.5 (2), we also have

$$
\Re \langle x, y \rangle \geq 0 \quad \text{and} \quad \Re \langle z, y \rangle \geq 0,
$$

from which we get

$$
\|v - u\|^2 = \|x + y + z\|^2 = \|x + z + y\|^2
$$

$$
= \|x + z\|^2 + \|y\|^2 + 2\Re \langle x, y \rangle + 2\Re \langle z, y \rangle
$$

$$
\geq \|y\|^2 = \|p_X(v) - p_X(u)\|^2.
$$

However, $\|p_X(v) - p_X(u)\| \leq \|v - u\|$ obviously implies that $p_X$ is continuous. \qed

We can now prove the following important proposition.

**Proposition 12.7.** Let $E$ be a Hilbert space.

(1) For any closed subspace $V \subseteq E$, we have $E = V \oplus V^\perp$, and the map $p_V : E \to V$ is linear and continuous.

(2) For any $u \in E$, the projection $p_V(u)$ is the unique vector $w \in E$ such that

$$
w \in V \quad \text{and} \quad \langle u - w, z \rangle = 0 \quad \text{for all } z \in V.$$
12.1. **The Projection Lemma, Duality**

![Figure 12.6: Let $X$ be the solid gold ellipsoid. The vector $v - u$ is the sum of the three green vectors, each of which is determined by the appropriate projections.](image)

**Proof.** (1) First, we prove that $u - p_V(u) \in V^\perp$ for all $u \in E$. For any $v \in V$, since $V$ is a subspace, $z = p_V(u) + \lambda v \in V$ for all $\lambda \in \mathbb{C}$, and since $V$ is convex and nonempty (since it is a subspace), and closed by hypothesis, by Proposition 29.5 (2), we have

$$\Re(\langle u - p_V(u), v \rangle) = \Re(\langle u - p_V(u), \lambda v \rangle) = \Re(\langle u - p_V(u), z - p_V(u) \rangle) \leq 0$$

for all $\lambda \in \mathbb{C}$. In particular, the above holds for $\lambda = \langle u - p_V(u), v \rangle$, which yields

$$|\langle u - p_V(u), v \rangle| \leq 0,$$

and thus, $\langle u - p_V(u), v \rangle = 0$. See Figure 29.7. As a consequence, $u - p_V(u) \in V^\perp$ for all $u \in E$. Since $u = p_V(u) + u - p_V(u)$ for every $u \in E$, we have $E = V + V^\perp$. On the other hand, since $\langle -, - \rangle$ is positive definite, $V \cap V^\perp = \{0\}$, and thus $E = V \oplus V^\perp$.

We already proved in Proposition 29.6 that $p_V : E \rightarrow V$ is continuous. Also, since

$$p_V(\lambda u + \mu v) - (\lambda p_V(u) + \mu p_V(v)) = p_V(\lambda u + \mu v) - (\lambda u + \mu v) + \lambda(u - p_V(u)) + \mu(v - p_V(v)),$$

for all $u, v \in E$, and since the left-hand side term belongs to $V$, and from what we just showed, the right-hand side term belongs to $V^\perp$, we have

$$p_V(\lambda u + \mu v) - (\lambda p_V(u) + \mu p_V(v)) = 0,$$

showing that $p_V$ is linear.

(2) This is basically obvious from (1). We proved in (1) that $u - p_V(u) \in V^\perp$, which is exactly the condition

$$\langle u - p_V(u), z \rangle = 0$$
for all $z \in V$. Conversely, if $w \in V$ satisfies the condition
\[
\langle u - w, z \rangle = 0
\]
for all $z \in V$, since $w \in V$, every vector $z \in V$ is of the form $y - w$, with $y = z + w \in V$, and thus, we have
\[
\langle u - w, y - w \rangle = 0
\]
for all $y \in V$, which implies the condition of Proposition 29.5 (2):
\[
\Re \langle u - w, y - w \rangle \leq 0
\]
for all $y \in V$. By Proposition 29.5, $w = p_V(u)$ is the projection of $u$ onto $V$. 

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure12_7}
\caption{Let $V$ be the pink plane. The vector $u - p_V(u)$ is perpendicular to any $v \in V$.}
\end{figure}

**Remark:** If $p_V : E \to V$ is linear, then $V$ is a subspace of $E$. It follows that if $V$ is a closed convex subset of $E$, then $p_V : E \to V$ is linear iff $V$ is a subspace of $E$.

Let us illustrate the power of Proposition 29.7 on the following “least squares” problem. Given a real $m \times n$-matrix $A$ and some vector $b \in \mathbb{R}^m$, we would like to solve the linear system
\[
Ax = b
\]
in the least-squares sense, which means that we would like to find some solution $x \in \mathbb{R}^n$ that minimizes the Euclidean norm $\|Ax - b\|$ of the error $Ax - b$. It is actually not clear that the problem has a solution, but it does! The problem can be restated as follows: Is there some $x \in \mathbb{R}^n$ such that
\[
\|Ax - b\| = \inf_{y \in \mathbb{R}^n} \|Ay - b\|,
\]
or equivalently, is there some $z \in \text{Im} (A)$ such that
\[\|z - b\| = d(b, \text{Im} (A)),\]
where $\text{Im} (A) = \{Ay \in \mathbb{R}^m \mid y \in \mathbb{R}^n\}$, the image of the linear map induced by $A$. Since $\text{Im} (A)$ is a closed subspace of $\mathbb{R}^m$, because we are in finite dimension, Proposition 29.7 tells us that there is a unique $z \in \text{Im} (A)$ such that
\[\|z - b\| = \inf_{y \in \mathbb{R}^n} \|Ay - b\|,
\]
and thus, the problem always has a solution since $z \in \text{Im} (A)$, and since there is at least some $x \in \mathbb{R}^n$ such that $Ax = z$ (by definition of $\text{Im} (A)$). Note that such an $x$ is not necessarily unique. Furthermore, Proposition 29.7 also tells us that $z \in \text{Im} (A)$ is the solution of the equation
\[\langle z - b, w \rangle = 0 \quad \text{for all} \quad w \in \text{Im} (A),\]
or equivalently, that $x \in \mathbb{R}^n$ is the solution of
\[\langle Ax - b, Ay \rangle = 0 \quad \text{for all} \quad y \in \mathbb{R}^n,
\]
which is equivalent to
\[\langle A^\top (Ax - b), y \rangle = 0 \quad \text{for all} \quad y \in \mathbb{R}^n,
\]
and thus, since the inner product is positive definite, to $A^\top (Ax - b) = 0$, i.e.,
\[A^\top Ax = A^\top b.
\]
Therefore, the solutions of the original least-squares problem are precisely the solutions of the so-called normal equations
\[A^\top Ax = A^\top b,
\]
discovered by Gauss and Legendre around 1800. We also proved that the normal equations always have a solution.

Computationally, it is best not to solve the normal equations directly, and instead, to use methods such as the QR-decomposition (applied to $A$) or the SVD-decomposition (in the form of the pseudo-inverse). We will come back to this point later on.

As another corollary of Proposition 29.7, for any continuous nonnull linear map $h: E \to \mathbb{C}$, the null space
\[H = \text{Ker} h = \{u \in E \mid h(u) = 0\} = h^{-1}(0)\]
is a closed hyperplane $H$, and thus, $H^\perp$ is a subspace of dimension one such that $E = H \oplus H^\perp$. This suggests defining the dual space of $E$ as the set of all continuous maps $h: E \to \mathbb{C}$.

**Remark:** If $h: E \to \mathbb{C}$ is a linear map which is not continuous, then it can be shown that the hyperplane $H = \text{Ker} h$ is dense in $E$! Thus, $H^\perp$ is reduced to the trivial subspace.
CHAPTER 12. BASICS OF HILBERT SPACES

{0}. This goes against our intuition of what a hyperplane in \( \mathbb{R}^n \) (or \( \mathbb{C}^n \)) is, and warns us not to trust our “physical” intuition too much when dealing with infinite dimensions. As a consequence, the map \( \flat: E \to E^* \) introduced in Section 12.2 (Vol. I) (see just after Definition 29.2 below) is not surjective, since the linear forms of the form \( u \mapsto \langle u, v \rangle \) (for some fixed vector \( v \in E \)) are continuous (the inner product is continuous).

We now show that by redefining the dual space of a Hilbert space as the set of continuous linear forms on \( E \), we recover Theorem 12.5 (Vol. I).

**Definition 12.2.** Given a Hilbert space \( E \), we define the dual space \( E' \) of \( E \) as the vector space of all continuous linear forms \( h: E \to \mathbb{C} \). Maps in \( E' \) are also called bounded linear operators, bounded linear functionals, or simply, operators or functionals.

As in Section 12.2 (Vol. I), for all \( u, v \in E \), we define the maps \( \varphi_u^l: E \to \mathbb{C} \) and \( \varphi_v^r: E \to \mathbb{C} \) such that

\[
\varphi_u^l(v) = \langle u, v \rangle,
\]

and

\[
\varphi_v^r(u) = \langle u, v \rangle.
\]

In fact, \( \varphi_u^l = \varphi_u^r \), and because the inner product \( \langle -, - \rangle \) is continuous, it is obvious that \( \varphi_v^r \) is continuous and linear, so that \( \varphi_v^r \in E' \). To simplify notation, we write \( \varphi_v \) instead of \( \varphi_v^r \).

Theorem 12.5 (Vol. I) is generalized to Hilbert spaces as follows.

**Proposition 12.8.** (Riesz representation theorem) Let \( E \) be a Hilbert space. Then, the map \( \flat: E \to E' \) defined such that

\[
\flat(v) = \varphi_v,
\]

is semilinear, continuous, and bijective. Furthermore, for any continuous linear map \( \psi \in E' \), if \( u \in E \) is the unique vector such that

\[
\psi(v) = \langle v, u \rangle \quad \text{for all } v \in E,
\]

then we have \( \|\psi\| = \|u\| \), where

\[
\|\psi\| = \sup \left\{ \frac{|\psi(v)|}{\|v\|} \middle| v \in E, \ v \neq 0 \right\}.
\]

**Proof.** The proof is basically identical to the proof of Theorem 12.5 (Vol. I), except that a different argument is required for the surjectivity of \( \flat: E \to E' \), since \( E \) may not be finite dimensional. For any nonnull linear operator \( h \in E' \), the hyperplane \( H = \text{Ker} \ h = h^{-1}(0) \) is a closed subspace of \( E \), and by Proposition 29.7, \( H^\perp \) is a subspace of dimension one such that \( E = H \oplus H^\perp \). Then, picking any nonnull vector \( w \in H^\perp \), observe that \( H \) is also the kernel of the linear operator \( \varphi_w \), with

\[
\varphi_w(u) = \langle u, w \rangle,
\]
and thus, since any two nonzero linear forms defining the same hyperplane must be propor-
tional, there is some nonzero scalar \( \lambda \in \mathbb{C} \) such that \( h = \lambda \varphi_w \). But then, \( h = \varphi_{\lambda w} \), proving that \( \varphi : E \to E' \) is surjective.

By the Cauchy–Schwarz inequality we have
\[
|\varphi(v)| = |\langle v, u \rangle| \leq \|v\| \|u\|,
\]
so by definition of \( \|\varphi\| \) we get
\[
\|\varphi\| \leq \|u\|.
\]
Obviously \( \varphi = 0 \) iff \( u = 0 \) so assume \( u \neq 0 \). We have
\[
\|u\|^2 = \langle u, u \rangle = \psi(u) \leq \|\varphi\| \|u\|,
\]
which yields \( \|u\| \leq \|\varphi\| \), and therefore \( \|\varphi\| = \|u\| \), as claimed. \( \square \)

Proposition 29.8 is known as the Riesz representation theorem, or “Little Riesz Theorem.” It shows that the inner product on a Hilbert space induces a natural semilinear isomorphism between \( E \) and its dual \( E' \) (equivalently, a linear isomorphism between \( \overline{E} \) and \( E' \)). This isomorphism is an isometry (it preserves the norm).

**Remark:** Many books on quantum mechanics use the so-called Dirac notation to denote objects in the Hilbert space \( E \) and operators in its dual space \( E' \). In the Dirac notation, an element of \( E \) is denoted as \( |x\rangle \), and an element of \( E' \) is denoted as \( \langle t| \). The scalar product is denoted as \( \langle t| \cdot |x\rangle \). This uses the isomorphism between \( E \) and \( E' \), except that the inner product is assumed to be semi-linear on the left, rather than on the right.

Proposition 29.8 allows us to define the adjoint of a linear map, as in the Hermitian case (see Proposition 12.6 (Vol. I)). Actually, we can prove a slightly more general result which is used in optimization theory.

If \( \varphi : E \times E \to \mathbb{C} \) is a sesquilinear map on a normed vector space \( (E, \|\|) \), then Proposition 19.17 is immediately adapted to prove that \( \varphi \) is continuous iff there is some constant \( k \geq 0 \) such that
\[
|\varphi(u, v)| \leq k \|u\| \|v\| \quad \text{for all } u, v \in E.
\]
Thus we define \( \|\varphi\| \) as in Definition 19.16 by
\[
\|\varphi\| = \sup \{|\varphi(x, y)| \mid \|x\| \leq 1, \|y\| \leq 1, \ x, y \in E\}.
\]

**Proposition 12.9.** Given a Hilbert space \( E \), for every continuous sesquilinear map \( \varphi : E \times E \to \mathbb{C} \), there is a unique continuous linear map \( f_\varphi : E \to E \), such that
\[
\varphi(u, v) = \langle u, f_\varphi(v) \rangle \quad \text{for all } u, v \in E.
\]
We also have \( \|f_\varphi\| = \|\varphi\| \). If \( \varphi \) is Hermitian, then \( f_\varphi \) is self-adjoint, that is
\[
\langle u, f_\varphi(v) \rangle = \langle f_\varphi(u), v \rangle \quad \text{for all } u, v \in E.
\]
Proof. The proof is adapted from Rudin [84] (Theorem 12.8). To define the function \( f_\varphi \) we proceed as follows. For any fixed \( v \in E \) define the linear map \( \varphi_v \) by

\[
\varphi_v(u) = \varphi(u, v) \quad \text{for all } u \in E.
\]

Since \( \varphi \) is continuous \( \varphi_v \) is continuous so by Proposition 29.8, there is a unique vector in \( E \) that we denote \( f_\varphi(v) \) such that

\[
\varphi_v(u) = \langle u, f_\varphi(v) \rangle \quad \text{for all } u \in E,
\]

and \( \|f_\varphi(v)\| = \|\varphi_v\| \). Let us check that the map \( v \mapsto f_\varphi(v) \) is linear.

We have

\[
\varphi(u, v_1 + v_2) = \varphi(u, v_1) + \varphi(u, v_2)
\]

\( \varphi \) is additive

\[
= \langle u, f_\varphi(v_1) \rangle + \langle u, f_\varphi(v_2) \rangle
\]

by definition of \( f_\varphi \)

\[
= \langle u, f_\varphi(v_1) + f_\varphi(v_2) \rangle
\]

\( \langle -, - \rangle \) is additive

for all \( u \in E \), and since \( f_\varphi(v_1 + v_2) \) is the unique vector such that \( \varphi(u, v_1 + v_2) = \langle u, f_\varphi(v_1 + v_2) \rangle \) for all \( u \in E \), we must have

\[
f_\varphi(v_1 + v_2) = f_\varphi(v_1) + f_\varphi(v_2).
\]

For any \( \lambda \in \mathbb{C} \) we have

\[
\varphi(u, \lambda v) = \overline{\lambda} \varphi(u, v)
\]

\( \varphi \) is sesquilinear

\[
= \overline{\lambda} \langle u, f_\varphi(v) \rangle
\]

by definition of \( f_\varphi \)

\[
= \langle u, \lambda f_\varphi(v) \rangle
\]

\( \langle -, - \rangle \) is sesquilinear

for all \( u \in E \), and since \( f_\varphi(\lambda v) \) is the unique vector such that \( \varphi(u, \lambda v) = \langle u, f_\varphi(\lambda v) \rangle \) for all \( u \in E \), we must have

\[
f_\varphi(\lambda v) = \lambda f_\varphi(v).
\]

Therefore \( f_\varphi \) is linear.

Then by definition of \( \|\varphi\| \) we have

\[
|\varphi_v(u)| = |\varphi(u, v)| \leq \|\varphi\| \|u\| \|v\|,
\]

which shows that \( \|\varphi_v\| \leq \|\varphi\| \|v\| \). Since \( \|f_\varphi(v)\| = \|\varphi_v\| \), we have

\[
\|f_\varphi(v)\| \leq \|\varphi\| \|v\|,
\]

which shows that \( f_\varphi \) is continuous and that \( \|f_\varphi\| \leq \|\varphi\| \). But by the Cauchy–Schwarz inequality we also have

\[
|\varphi(u, v)| = |\langle u, f_\varphi(v) \rangle| \leq \|u\| \|f_\varphi(v)\| \leq \|u\| \|f_\varphi\| \|v\|,
\]
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so \( \|\varphi\| \leq \|f\varphi\| \), and thus

\[
\|f\varphi\| = \|\varphi\|.
\]

If \( \varphi \) is Hermitian, \( \varphi(v, u) = \overline{\varphi(u, v)} \), so

\[
\langle f\varphi(u), v \rangle = \langle v, f\varphi(u) \rangle = \overline{\varphi(v, u)} = \varphi(u, v) = \langle u, f\varphi(v) \rangle,
\]

which shows that \( f\varphi \) is self-adjoint. \( \square \)

**Proposition 12.10.** Given a Hilbert space \( E \), for every continuous linear map \( f : E \to E \), there is a unique continuous linear map \( f^* : E \to E \), such that

\[
\langle f(u), v \rangle = \langle u, f^*(v) \rangle \quad \text{for all } u, v \in E,
\]

and we have \( \|f^*\| = \|f\| \). The map \( f^* \) is called the adjoint of \( f \).

**Proof.** The proof is adapted from Rudin [84] (Section 12.9). By the Cauchy–Schwarz inequality

\[
|\langle x, y \rangle| \leq \|x\| \|y\|
\]

we see that the sesquilinear map \( (x, y) \mapsto \langle x, y \rangle \) on \( E \times E \) is continuous. Let \( \varphi : E \times E \to \mathbb{C} \) be the sesquilinear map given by

\[
\varphi(u, v) = \langle f(u), v \rangle \quad \text{for all } u, v \in E.
\]

Since \( f \) is continuous and the inner product \( \langle -, - \rangle \) is continuous, this is a continuous map. By Proposition 29.9 there is a unique linear map \( f^* : E \to E \) such that

\[
\langle f(u), v \rangle = \varphi(u, v) = \langle u, f^*(v) \rangle \quad \text{for all } u, v \in E,
\]

with \( \|f^*\| = \|\varphi\| \).

We can also prove that \( \|\varphi\| = \|f\| \). First, by definition of \( \|\varphi\| \) we have

\[
\|\varphi\| = \sup \{ |\varphi(x, y)| \mid \|x\| \leq 1, \|y\| \leq 1 \} \\
= \sup \{ \|\langle f(x), y \rangle\| \mid \|x\| \leq 1, \|y\| \leq 1 \} \\
\leq \sup \{ \|\langle f(x)\| \|y\| \| \mid \|x\| \leq 1, \|y\| \leq 1 \} \\
\leq \sup \{ \|f(x)\| \|y\| \| \mid \|x\| \leq 1 \} \\
= \|f\|.
\]

In the other direction we have

\[
\|f(x)\|^2 = \langle f(x), f(x) \rangle = \varphi(x, f(x)) \leq \|\varphi\| \|x\| \|f(x)\|,
\]

and if \( f(x) \neq 0 \) we get \( \|f(x)\| \leq \|\varphi\||\|x\| \). This inequality holds trivially if \( f(x) = 0 \), so we conclude that \( \|f\| \leq \|\varphi\| \). Therefore we have

\[
\|\varphi\| = \|f\|,
\]

as claimed, and consequently \( \|f^*\| = \|\varphi\| = \|f\| \). \( \square \)
It is easy to show that the adjoint satisfies the following properties:

\[
(f + g)^* = f^* + g^*
\]
\[
(\lambda f)^* = \overline{\lambda} f^*
\]
\[
(f \circ g)^* = g^* \circ f^*
\]
\[
f^{**} = f.
\]

One can also show that \(\|f^* \circ f\| = \|f\|^2\) (see Rudin [84], Section 12.9).

As in the Hermitian case, given two Hilbert spaces \(E\) and \(F\), the above results can be adapted to show that for any linear map \(f: E \to F\), there is a unique linear map \(f^*: F \to E\) such that

\[
\langle f(u), v \rangle_2 = \langle u, f^*(v) \rangle_1
\]
for all \(u \in E\) and all \(v \in F\). The linear map \(f^*\) is also called the adjoint of \(f\).

### 12.2 Farkas–Minkowski Lemma in Hilbert Spaces

In this section, \((V, \langle - , - \rangle)\) is assumed to be a real Hilbert space. The projection lemma can be used to show an interesting version of the Farkas–Minkowski lemma in a Hilbert space.

Given a finite sequence of vectors \((a_1, \ldots, a_m)\) with \(a_i \in V\), let \(C\) be the polyhedral cone

\[
C = \text{cone}(a_1, \ldots, a_m) = \left\{ \sum_{i=1}^{m} \lambda_i a_i \mid \lambda_i \geq 0, \ i = 1, \ldots, m \right\}.
\]

For any vector \(b \in V\), the Farkas–Minkowski lemma gives a criterion for checking whether \(b \in C\).

In Proposition 25.2 we proved that every polyhedral cone \(\text{cone}(a_1, \ldots, a_m)\) with \(a_i \in \mathbb{R}^n\) is closed. Close examination of the proof shows that it goes through if \(a_i \in V\) where \(V\) is any vector space possibly of infinite dimension, because the important fact is that the number \(m\) of these vectors is finite, not their dimension.

**Theorem 12.11.** (Farkas–Minkowski Lemma in Hilbert Spaces) Let \((V, \langle - , - \rangle)\) be a real Hilbert space. For any finite sequence of vectors \((a_1, \ldots, a_m)\) with \(a_i \in V\), if \(C\) is the polyhedral cone \(C = \text{cone}(a_1, \ldots, a_m)\), for any vector \(b \in V\), we have \(b \notin C\) iff there is a vector \(u \in V\) such that

\[
\langle a_i, u \rangle \geq 0 \quad i = 1, \ldots, m, \quad \text{and} \quad \langle b, u \rangle < 0.
\]

Equivalently, \(b \in C\) iff for all \(u \in V\),

\[
\text{if } \langle a_i, u \rangle \geq 0 \quad i = 1, \ldots, m, \quad \text{then} \quad \langle b, u \rangle \geq 0.
\]
Proof. We follow Ciarlet [30] (Chapter 9, Theorem 9.1.1). We already established in Proposition 25.2 that the polyhedral cone $C = \text{cone}(a_1, \ldots, a_m)$ is closed. Next we claim the following:

Claim: If $C$ is a nonempty, closed, convex subset of a Hilbert space $V$, and $b \in V$ is any vector such that $b \notin C$, then there exist some $u \in V$ and infinitely many scalars $\alpha \in \mathbb{R}$ such that

$$\langle v, u \rangle > \alpha \quad \text{for every } v \in C$$
$$\langle b, u \rangle < \alpha.$$

We use the projection lemma (Proposition 29.5) which says that since $b \notin C$ there is some unique $c = p_C(b) \in C$ such that

$$\|b - c\| = \inf_{v \in C} \|b - v\| > 0$$
$$\langle b - c, v - c \rangle \leq 0 \quad \text{for all } v \in C,$$

or equivalently

$$\|b - c\| = \inf_{v \in C} \|b - v\| > 0$$
$$\langle v - c, c - b \rangle \geq 0 \quad \text{for all } v \in C.$$

As a consequence we have

$$\langle v, c - b \rangle \geq \langle c, c - b \rangle > \langle b, c - b \rangle,$$

and if we pick $u = c - b$ and any $\alpha$ such that

$$\langle c, c - b \rangle > \alpha > \langle b, c - b \rangle,$$

the claim is satisfied.

We now prove the Farkas–Minkowski Lemma. Assume that $b \notin C$. Since $C$ is nonempty, convex, and closed, by the Claim there is some $u \in V$ and some $\alpha \in \mathbb{R}$ such that

$$\langle v, u \rangle > \alpha \quad \text{for every } v \in C$$
$$\langle b, u \rangle < \alpha.$$

But $C$ is a polyhedral cone containing 0 so we must have $\alpha < 0$. Then for every $v \in C$, since $C$ a polyhedral cone if $v \in C$ then $\lambda v \in C$ for all $\lambda > 0$, so by the above

$$\langle v, u \rangle > \frac{\alpha}{\lambda} \quad \text{for every } \lambda > 0,$$

which implies that

$$\langle v, u \rangle \geq 0.$$

Since $a_i \in C$ for $i = 1, \ldots, m$, we proved that

$$\langle a_i, u \rangle \geq 0 \quad i = 1, \ldots, m \quad \text{and} \quad \langle b, u \rangle < \alpha < 0,$$

which proves Farkas Lemma.
Observe that the claim established during the proof of Theorem 29.11 shows that the affine hyperplane $H_{u,\alpha}$ of equation $\langle v, u \rangle = \alpha$ for all $v \in V$ separates strictly $C$ and $\{b\}$. 
Chapter 13
General Results of Optimization Theory

13.1 Existence of Solutions of an Optimization Problem

The main goal of optimization theory is to construct algorithms to find solutions (often approximate) of problems of the form

\[
\text{find} \quad u \quad \text{such that} \quad u \in U \quad \text{and} \quad J(u) = \inf_{v \in U} J(v),
\]

where \( U \) is a given subset of a vector space \( V \) (possibly infinite dimensional) and \( J: \Omega \to \mathbb{R} \) is a function defined on some open subset \( \Omega \) of \( V \) such that \( U \subseteq \Omega \).

To be very clear, \( \inf_{v \in U} J(v) \) denotes the greatest lower bound of the set of real number \( \{J(u) \mid u \in U\} \). To make sure that we are on firm grounds let us review the notions of greatest lower bound and least upper bound of a set of real numbers.

Let \( X \) be any nonempty subset of \( \mathbb{R} \). The set \( LB(X) \) of lower bounds of \( X \) is defined as

\[
LB(X) = \{b \in \mathbb{R} \mid b \leq x \text{ for all } x \in X\}.
\]

If the set \( X \) is not bounded below, which means that for every \( r \in \mathbb{R} \) there is some \( x \in X \) such that \( x < r \), then \( LB(X) \) is empty. Otherwise, if \( LB(X) \) is nonempty, since it is bounded above by every element of \( X \), by a fundamental property of the real numbers, the set \( LB(X) \) has a greatest element denoted \( \inf X \). The real number \( \inf X \) is thus the greatest lower bound of \( X \). In general, \( \inf X \) does not belong to \( X \), but if it does, then it is the least element of \( X \).

If \( LB(X) = \emptyset \), then \( X \) is unbounded below and \( \inf X \) is undefined. In this case (with an abuse of notation), we write

\[
\inf X = -\infty.
\]
By convention, when \( X = \emptyset \) we set
\[
\inf \emptyset = +\infty.
\]

Similarly the set \( UB(X) \) of upper bounds of \( X \) is given by
\[
UB(X) = \{ u \in \mathbb{R} \mid x \leq u \text{ for all } x \in X \}.
\]

If \( X \) is not bounded above, then \( UB(X) = \emptyset \). Otherwise, if \( UB(X) \neq \emptyset \), then it has least element denoted \( \sup X \). Thus \( \sup X \) is the least upper bound of \( X \). If \( \sup X \in X \), then it is the greatest element of \( X \). If \( UB(X) = \emptyset \), then \( \sup X = +\infty \).

By convention, when \( X = \emptyset \) we set
\[
\sup \emptyset = -\infty.
\]

The element \( \inf_{v \in U} J(v) \) is just \( \inf \{ J(v) \mid v \in U \} \). The notation \( J^* \) is often used to denote \( \inf_{v \in U} J(v) \). If the function \( J \) is not bounded below, which means that for every \( r \in \mathbb{R} \), there is some \( u \in U \) such that \( J(u) < r \), then
\[
\inf_{v \in U} J(v) = -\infty,
\]
and we say that our minimization problem has no solution, or that it is unbounded (below). For example, if \( V = \Omega = \mathbb{R} \), \( U = \{ x \in \mathbb{R} \mid x \leq 0 \} \), and \( J(x) = -x \), then the function \( J(x) \) is not bounded below and \( \inf_{v \in U} J(v) = -\infty \).

The issue is that \( J^* \) may not belong to \( \{ J(u) \mid u \in U \} \), that is, it may not be achieved by some element \( u \in U \), and solving the above problem consists in finding some \( u \in U \) that achieves the value \( J^* \) in the sense that \( J(u) = J^* \). If no such \( u \in U \) exists, again we say that our minimization problem has no solution.

The minimization problem
\[
\text{find } u \text{ such that } u \in U \text{ and } J(u) = \inf_{v \in U} J(v)
\]
is often presented in the following more informal way:

\[
\begin{align*}
\text{minimize} & \quad J(v) \\
\text{subject to} & \quad v \in U.
\end{align*}
\]

A vector \( u \in U \) such that \( J(u) = \inf_{v \in U} J(v) \) is often called a minimizer of \( J \) over \( U \). Some authors denote the set of minimizers of \( J \) over \( U \) by \( \arg \min_{v \in U} J(v) \) and write
\[
u \in \arg \min_{v \in U} J(v)\]
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to express that \( u \) is such a minimizer. When such a minimizer is unique, by abuse of notation, this unique minimizer \( u \) is denoted by

\[
\begin{align*}
  u &= \arg \min_{v \in U} J(v) .
\end{align*}
\]

We prefer not to use this notation, although it seems to have invaded the literature.

If we need to maximize rather than minimize a function, then we try to find some \( u \in U \) such that

\[
\begin{align*}
  J(u) &= \sup_{v \in U} J(v) .
\end{align*}
\]

Here \( \sup_{v \in U} J(v) \) is the least upper bound of the set \( \{ J(u) \mid u \in U \} \). Some authors denote the set of maximizers of \( J \) over \( U \) by \( \arg \max_{v \in U} J(v) \).

**Remark:** Some authors define an extended real-valued function as a function \( f : \Omega \to \mathbb{R} \) which is allowed to take the value \(-\infty\) or even \(+\infty\) for some of its arguments. Although this may be convenient to deal with situations where we need to consider \( \inf_{v \in U} J(v) \) or \( \sup_{v \in U} J(v) \), such “functions” are really partial functions and we prefer not to use the notion of extended real-valued function.

In most cases, \( U \) is defined as the set of solutions of a finite sets of constraints, either equality constraints \( \varphi_i(v) = 0 \), or inequality constraints \( \varphi_i(v) \leq 0 \), where the \( \varphi_i : \Omega \to \mathbb{R} \) are some given functions. The function \( J \) is often called the functional of the optimization problem. This is a slightly odd terminology, but it is justified if \( V \) is a function space.

The following questions arise naturally:

1. Results concerning the existence and uniqueness of a solution of the above problem. In the next section we state sufficient conditions either on the domain \( U \) or on the function \( J \) that ensure the existence of a solution.

2. The characterization of the possible solutions of the above problem. These are conditions for any element \( u \in U \) to be a solution of the problem. Such conditions usually involve the derivative \( dJ_u \) of \( J \), and possibly the derivatives of the functions \( \varphi_i \) defining \( U \). Some of these conditions become sufficient when the functions \( \varphi_i \) are convex.

3. The effective construction of algorithms, typically iterative algorithms that construct a sequence \( (u_k)_{k \geq 1} \) of elements of \( U \) whose limit is a solution \( u \in U \) of our problem. It is then necessary to understand when and how quickly such sequences converge. Gradient descent methods fall under this category. As a general rule, unconstrained problems (for which \( U = \Omega = V \)) are (much) easier to deal with than constrained problems (where \( U \neq V \)).

The material of this chapter is heavily inspired by Ciarlet [30]. In this chapter it is assumed that \( V \) is a real vector space with an inner product \( \langle -, - \rangle \). If \( V \) is infinite dimensional, then we assume that it is a real Hilbert space (it is complete). As usual, we write
∥u∥ = ⟨u, u⟩^{1/2} for the norm associated with the inner product ⟨−, −⟩. The reader may want to review Section 29.1, especially the projection lemma and the Riesz representation theorem.

As a matter of terminology, if \( U \) is defined by inequality and equality constraints as
\[
U = \{ v \in \Omega \mid \varphi_i(v) \leq 0, \ i = 1, \ldots, m, \ \psi_j(v) = 0, \ j = 1, \ldots, p \},
\]
if \( J \) and all the functions \( \varphi_i \) and \( \psi_j \) are affine, the problem is said to be \textit{linear} (or a \textit{linear program}), and otherwise \textit{nonlinear}. If \( J \) is of the form
\[
J(v) = \langle Av, v \rangle - \langle b, v \rangle
\]
where \( A \) is a nonzero symmetric positive semidefinite matrix and the constraints are affine, the problem is called a \textit{quadratic programming problem}.

We begin with the case where \( U \) is a closed but possibly unbounded subset of \( \mathbb{R}^n \). In this case the following type of functions arise.

**Definition 13.1.** A real-valued function \( J : V \to \mathbb{R} \) defined on a normed vector space \( V \) is \textit{coercive} iff for any sequence \( (v_k)_{k \geq 1} \) of vectors \( v_k \in V \), if \( \lim_{k \to \infty} \|v_k\| = \infty \), then
\[
\lim_{k \to \infty} J(v_k) = +\infty.
\]

For example, the function \( f(x) = x^2 + 2x \) is coercive, but an affine function \( f(x) = ax + b \) is not.

**Proposition 13.1.** Let \( U \) be a nonempty, closed subset of \( \mathbb{R}^n \), and let \( J : \mathbb{R}^n \to \mathbb{R} \) be a continuous function which is coercive if \( U \) is unbounded. Then there is a least one element \( u \in \mathbb{R}^n \) such that
\[
u \in U \quad \text{and} \quad J(u) = \inf_{v \in U} J(v).
\]

**Proof.** Since \( U \neq \emptyset \), pick any \( u_0 \in U \). Since \( J \) is coercive, there is some \( r > 0 \) such that for all \( v \in V \), if \( \|v\| > r \) then \( J(u_0) < J(v) \). It follows that \( J \) is minimized over the set
\[
U_0 = U \cap \{ v \in \mathbb{R}^n \mid \|v\| \leq r \}.
\]

Since \( U \) is closed and since the closed ball \( \{ v \in \mathbb{R}^n \mid \|v\| \leq r \} \) is compact, \( U_0 \) is compact, but we know that any continuous function on a compact set has a minimum which is achieved. \( \square \)

The key point in the above proof is the fact that \( U_0 \) is compact. In order to generalize Proposition 30.1 to the case of an infinite dimensional vector space, we need some additional assumptions, and it turns out that the convexity of \( U \) and of the function \( J \) is sufficient. The key is that convex, closed and bounded subsets of a Hilbert space are “weakly compact.”
Definition 13.2. Let $V$ be a Hilbert space. A sequence $(u_k)_{k \geq 1}$ of vectors $u_k \in V$ converges weakly if there is some $u \in V$ such that
\[ \lim_{k \to \infty} \langle v, u_k \rangle = \langle v, u \rangle \quad \text{for every } v \in V. \]

Recall that a Hilbert space is separable if it has a countable Hilbert basis (see Definition A.4). Also, in a Euclidean space $V$ the inner product induces an isomorphism between $V$ and its dual $V^*$. In our case, we need the isomorphism $\sharp$ from $V^*$ to $V$ defined such that for every linear form $\omega \in V^*$, the vector $\omega \sharp \in V$ is uniquely defined by the equation
\[ \omega(v) = \langle v, \omega \sharp \rangle \quad \text{for all } v \in V. \]

In a Hilbert space, the dual space $V'$ is the set of all continuous linear forms $\omega: V \to \mathbb{R}$, and the existence of the isomorphism $\sharp$ between $V'$ and $V$ is given by the Riesz representation theorem; see Proposition 29.8. This theorem allows a generalization of the notion of gradient. Indeed, if $f: V \to \mathbb{R}$ is a function defined on the Hilbert space $V$ and if $f$ is differentiable at some point $u \in V$, then by definition, the derivative $df_u: V \to \mathbb{R}$ is a continuous linear form, so by the Riesz representation theorem (Proposition 29.8) there is a unique vector, denoted $\nabla f_u \in V$, such that
\[ df_u(v) = \langle v, \nabla f_u \rangle \quad \text{for all } v \in V. \]
By definition, the vector $\nabla f_u$ is the gradient of $f$ at $u$.

Similarly, since the second derivative $D^2 f_u: V \to V'$ of $f$ induces a continuous symmetric bilinear form from $V \times V$ to $\mathbb{R}$, by Proposition 29.9, there is a unique continuous self-adjoint linear map $\nabla^2 f_u: V \to V$ such that
\[ D^2 f_u(v, w) = \langle \nabla^2 f_u(v), w \rangle \quad \text{for all } v, w \in V. \]

The map $\nabla^2 f_u$ is a generalization of the Hessian.

The next theorem is a rather general result about the existence of minima of convex functions defined on convex domains. The proof is quite involved and can be omitted upon first reading.

Theorem 13.2. Let $U$ be a nonempty, convex, closed subset of a separable Hilbert space $V$, and let $J: V \to \mathbb{R}$ be a convex, differentiable function which is coercive if $U$ is unbounded. Then there is a least one element $u \in V$ such that
\[ u \in U \quad \text{and} \quad J(u) = \inf_{v \in U} J(v). \]

Proof. As in the proof of Proposition 30.1, since the function $J$ is coercive, we may assume that $U$ is bounded and convex (however, if $V$ infinite dimensional, then $U$ is not compact in general). The proof proceeds in four steps.
Step 1. Consider a minimizing sequence \((u_k)_{k \geq 0}\), namely a sequence of elements \(u_k \in V\) such that
\[
u_k \in U \quad \text{for all } k \geq 0, \quad \lim_{k \to \infty} J(u_k) = \inf_{v \in U} J(v).
\]
At this stage, it is possible that \(\inf_{v \in U} J(v) = -\infty\), but we will see that this is actually impossible. However, since \(U\) is bounded, the sequence \((u_k)_{k \geq 0}\) is bounded. Our goal is to prove that there is some subsequence of \((w_\ell)_{\ell \geq 0}\) of \((u_k)_{k \geq 0}\) that converges weakly.

Since the sequence \((u_k)_{k \geq 0}\) is bounded there is some constant \(C > 0\) such that \(\|u_k\| \leq C\) for all \(k \geq 0\). Then, by the Cauchy–Schwarz inequality, for every \(v \in V\) we have
\[
|\langle v, u_k \rangle| \leq \|v\| \|u_k\| \leq C \|v\|,
\]
which shows that the sequence \((\langle v, u_k \rangle)_{k \geq 0}\) is bounded. Since \(V\) is a separable Hilbert space, there is a countable family \((v_k)_{k \geq 0}\) of vectors \(v_k \in V\) which is dense in \(V\). Since the sequence \((\langle v_1, u_k \rangle)_{k \geq 0}\) is bounded (in \(\mathbb{R}\)), we can find a convergent subsequence \((\langle v_1, u_{i_1}(j) \rangle)_{j \geq 0}\). Similarly, since the sequence \((\langle v_2, u_{i_2}(j) \rangle)_{j \geq 0}\) is bounded, we can find a convergent subsequence \((\langle v_2, u_{i_2(j)} \rangle)_{j \geq 0},\) and in general, since the sequence \((\langle v_k, u_{i_k-1}(j) \rangle)_{j \geq 0}\) is bounded, we can find a convergent subsequence \((\langle v_k, u_{i_k(j)} \rangle)_{j \geq 0}\).

We obtain the following infinite array:
\[
\begin{pmatrix}
\langle v_1, u_{i_1(1)} \rangle & \langle v_2, u_{i_2(1)} \rangle & \cdots & \langle v_k, u_{i_k(1)} \rangle & \cdots \\
\langle v_1, u_{i_1(2)} \rangle & \langle v_2, u_{i_2(2)} \rangle & \cdots & \langle v_k, u_{i_k(2)} \rangle & \cdots \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
\langle v_1, u_{i_1(k)} \rangle & \langle v_2, u_{i_2(k)} \rangle & \cdots & \langle v_k, u_{i_k(k)} \rangle & \cdots \\
\vdots & \vdots & \ddots & \vdots & \vdots
\end{pmatrix}
\]
Consider the “diagonal” sequence \((w_\ell)_{\ell \geq 0}\) defined by
\[
w_\ell = u_{i_\ell(\ell)}, \quad \ell \geq 0.
\]
We are going to prove that for every \(v \in V\), the sequence \((\langle v, w_\ell \rangle)_{\ell \geq 0}\) has a limit.

By construction, for every \(k \geq 0\), the sequence \((\langle v_k, w_\ell \rangle)_{\ell \geq 0}\) has a limit, which is the limit of the sequence \((\langle v_k, u_{i_k(j)} \rangle)_{j \geq 0}\), since the sequence \((i_\ell(\ell))_{\ell \geq 0}\) is a subsequence of every sequence \((i_\ell(j))_{j \geq 0}\) for every \(\ell \geq 0\).

Pick any \(v \in V\) and any \(\epsilon > 0\). Since \((v_k)_{k \geq 0}\) is dense in \(V\), there is some \(v_k\) such that
\[
\|v - v_k\| \leq \epsilon/(4C).
\]
Then we have
\[
|\langle v, w_\ell \rangle - \langle v, w_m \rangle| = |\langle v, w_\ell - w_m \rangle|
= |\langle v_k + v - v_k, w_\ell - w_m \rangle|
= |\langle v_k, w_\ell - w_m \rangle + \langle v - v_k, w_\ell - w_m \rangle|
\leq |\langle v_k, w_\ell \rangle - \langle v_k, w_m \rangle| + |\langle v - v_k, w_\ell - w_m \rangle|.
\]
By Cauchy–Schwarz and since $\|w_\ell - w_m\| \leq \|w_\ell\| + \|w_m\| \leq C + C = 2C$,

$$|\langle v - v_k, w_\ell - w_m \rangle| \leq \|v - v_k\| \|w_\ell - w_m\| \leq (\varepsilon/(4C))2C = \varepsilon/2,$$

so

$$|\langle v, w_\ell \rangle - \langle v, w_m \rangle| \leq |\langle v_k, w_\ell - w_m \rangle| + \varepsilon/2.$$

With the element $v_k$ held fixed, by a previous argument the sequence $(\langle v_k, w_\ell \rangle)_{\ell \geq 0}$ converges, so it is a Cauchy sequence. Consequently there is some $\ell_0$ (depending on $\varepsilon$ and $v_k$) such that

$$|\langle v_k, w_\ell \rangle - \langle v_k, w_m \rangle| \leq \varepsilon/2 \quad \text{for all } \ell, m \geq \ell_0,$$

so we get

$$|\langle v, w_\ell \rangle - \langle v, w_m \rangle| \leq \varepsilon/2 + \varepsilon/2 = \varepsilon \quad \text{for all } \ell, m \geq \ell_0.$$

This proves that the sequence $(\langle v, w_\ell \rangle)_{\ell \geq 0}$ is a Cauchy sequence, and thus it converges.

Define the function $g : V \to \mathbb{R}$ by

$$g(v) = \lim_{\ell \to \infty} \langle v, w_\ell \rangle, \quad \text{for all } v \in V.$$

Since

$$|\langle v, w_\ell \rangle| \leq \|v\| \|w_\ell\| \leq C \|v\| \quad \text{for all } \ell \geq 0,$$

we have

$$|g(v)| \leq C \|v\|,$$

so $g$ is a continuous linear map. By the Riesz representation theorem (Proposition 29.8), there is a unique $u \in V$ such that

$$g(v) = \langle v, u \rangle \quad \text{for all } v \in V,$$

which shows that

$$\lim_{\ell \to \infty} \langle v, w_\ell \rangle = \langle v, u \rangle \quad \text{for all } v \in V,$$

namely the subsequence $(w_\ell)_{\ell \geq 0}$ of the sequence $(u_k)_{k \geq 0}$ converges weakly to $u \in V$.

**Step 2.** We prove that the “weak limit” $u$ of the sequence $(w_\ell)_{\ell \geq 0}$ belongs to $U$.

Consider the projection $p_U(u)$ of $u \in V$ onto the closed convex set $U$. Since $w_\ell \in U$, by Proposition 29.5 we have

$$\langle p_U(u) - u, w_\ell - p_U(u) \rangle \geq 0 \quad \text{for all } \ell \geq 0.$$

The weak convergence of the sequence $(w_\ell)_{\ell \geq 0}$ to $u$ implies that

$$0 \leq \lim_{\ell \to \infty} \langle p_U(u) - u, w_\ell - p_U(u) \rangle = \langle p_U(u) - u, u - p_U(u) \rangle = -\|p_U(u) - u\| \leq 0,$$
so \( \| p_U(u) - u \| = 0 \), which means that \( p_U(u) = u \), and so \( u \in U \).

**Step 3.** We prove that

\[
J(v) \leq \liminf_{\ell \to \infty} J(z_\ell)
\]

for every sequence \((z_\ell)_{\ell \geq 0}\) converging weakly to some element \(v \in V\).

Since \( J \) is assumed to be differentiable and convex, by Proposition 21.9 we have

\[
J(v) + \langle \nabla J_v, z_\ell - v \rangle \leq J(z_\ell) \quad \text{for all } \ell \geq 0,
\]

and by definition of weak convergence

\[
\lim_{\ell \to \infty} \langle \nabla J_v, z_\ell \rangle = \langle \nabla J_v, v \rangle,
\]

so \( \lim_{\ell \to \infty} \langle \nabla J_v, z_\ell - v \rangle = 0 \), and by definition of \( \liminf \) we get

\[
J(v) \leq \liminf_{\ell \to \infty} J(z_\ell)
\]

for every sequence \((z_\ell)_{\ell \geq 0}\) converging weakly to some element \(v \in V\).

**Step 4.** The weak limit \( u \in U \) of the subsequence \((w_\ell)_{\ell \geq 0}\) extracted from the minimizing sequence \((u_k)_{k \geq 0}\) satisfies the equation

\[
J(u) = \inf_{v \in U} J(v).
\]

By Step (1) and Step (2) the subsequence \((w_\ell)_{\ell \geq 0}\) of the sequence \((u_k)_{k \geq 0}\) converges weakly to some element \(u \in U\), so by Step (3) we have

\[
J(u) \leq \liminf_{\ell \to \infty} J(w_\ell).
\]

On the other hand, by definition of \((w_\ell)_{\ell \geq 0}\) as a subsequence of \((u_k)_{k \geq 0}\), since the sequence \((J(u_k))_{k \geq 0}\) converges to \(J(v)\), we have

\[
J(u) \leq \liminf_{\ell \to \infty} J(w_\ell) = \lim_{k \to \infty} J(u_k) = \inf_{v \in U} J(v),
\]

which proves that \( u \in U \) achieves the minimum of \( J \) on \( U \).

**Remark:** Theorem 30.2 still holds if we only assume that \( J \) is convex and continuous. It also holds in a reflexive Banach space, of which Hilbert spaces are a special case; see Brezis [24], Corollary 3.23.

Theorem 30.2 is a rather general theorem whose proof is quite involved. For functions \( J \) of a certain type, we can obtain existence and uniqueness results that are easier to prove. This is true in particular for quadratic functionals.
**Definition 13.3.** Let $V$ be a real Hilbert space. A function $J: V \to \mathbb{R}$ is called a *quadratic functional* if it is of the form

$$J(v) = \frac{1}{2}a(v, v) - h(v),$$

where $a: V \times V \to \mathbb{R}$ is a bilinear form which is symmetric and continuous, and $h: V \to \mathbb{R}$ is a continuous linear form.

Definition 30.3 is a natural extension of the notion of a quadratic functional on $\mathbb{R}^n$. Indeed, by Proposition 29.9, there is a unique continuous self-adjoint linear map $A: V \to V$ such that

$$a(u, v) = \langle Au, v \rangle \quad \text{for all } u, v \in V,$$

and by the Riesz representation theorem (Proposition 29.8), there is a unique $b \in V$ such that

$$h(v) = \langle b, v \rangle \quad \text{for all } v \in V.$$

Consequently, $J$ can be written as

$$J(v) = \frac{1}{2}\langle Av, v \rangle - \langle b, v \rangle \quad \text{for all } v \in V.$$

Since $a$ is bilinear and $h$ is linear, observe that the derivative of $J$ is given by

$$dJ_u(v) = a(u, v) - h(v) \quad \text{for all } v \in V,$$

or equivalently by

$$dJ_u(v) = \langle Au, v \rangle - \langle b, v \rangle = \langle Au - b, v \rangle, \quad \text{for all } v \in V.$$

Thus the gradient of $J$ is given by

$$\nabla J_u = Au - b,$$

just as in the case of a quadratic function of the form $J(v) = (1/2)v^TAv - b^Tv$, where $A$ is a symmetric $n \times n$ matrix and $b \in \mathbb{R}^n$. To find the second derivative $D^2J_u$ of $J$ at $u$ we compute

$$dJ_{u+v}(w) - dJ_u(w) = a(u + v, w) - h(w) - (a(u, w) - h(w)) = a(v, w),$$

so

$$D^2J_u(v, w) = a(v, w) = \langle Av, w \rangle,$$

which yields

$$\nabla^2J_u = A.$$

We will also make use of the following formula (if $J$ is a quadratic functional):

$$J(u + \rho v) = \frac{\rho^2}{2}a(v, v) + \rho(a(u, v) - h(v)) + J(u).$$
Indeed, since $a$ is symmetric bilinear and $h$ is linear, we have

\[ J(u + \rho v) = \frac{1}{2} a(u + \rho v, u + \rho v) - h(u + \rho v) \]

\[
\frac{\rho^2}{2} a(v, v) + \rho a(u, v) + \frac{1}{2} a(u, u) - h(u) - \rho h(v)
\]

\[ = \frac{\rho^2}{2} a(v, v) + \rho (a(u, v) - h(v)) + J(u). \]

Since $dJ_u(v) = a(u, v) - h(v) = \langle Au - b, v \rangle$ and $\nabla J_u = Au - b$, we can also write

\[ J(u + \rho v) = \frac{\rho^2}{2} a(v, v) + \rho \langle \nabla J_u, v \rangle + J(u). \]

We have the following theorem about the existence and uniqueness of minima of quadratic functionals.

**Theorem 13.3.** Given any Hilbert space $V$, let $J : V \to \mathbb{R}$ be a quadratic functional of the form

\[ J(v) = \frac{1}{2} a(v, v) - h(v). \]

Assume that there is some real number $\alpha > 0$ such that

\[ a(v, v) \geq \alpha \|v\|^2 \quad \text{for all } v \in V. \quad (\ast_\alpha) \]

If $U$ is any nonempty, closed, convex subset of $V$, then there is a unique $u \in U$ such that

\[ J(u) = \inf_{v \in U} J(v). \]

The element $u \in U$ satisfies the condition

\[ a(u, v - u) \geq h(v - u) \quad \text{for all } v \in U. \quad (*) \]

Conversely, if an element $u \in U$ satisfies $(*)$, then

\[ J(u) = \inf_{v \in U} J(v). \]

If $U$ is a subspace of $V$, then the above inequalities are replaced by the equations

\[ a(u, v) = h(v) \quad \text{for all } v \in U. \quad (\ast \ast) \]

**Proof.** The key point is that the bilinear form $a$ is actually an inner product in $V$. This is because it is positive definite, since $(\ast_\alpha)$ implies that

\[ \sqrt{\alpha} \|v\| \leq (a(v, v))^{1/2}, \]
and on the other hand the continuity of \( a \) implies that
\[
a(v, v) \leq \|a\| \|v\|^2,
\]
so we get
\[
\sqrt{\alpha} \|v\| \leq (a(v, v))^{1/2} \leq \sqrt{\|a\|} \|v\|.
\]
The above also shows that the norm \( v \mapsto (a(v, v))^{1/2} \) induced by the inner product \( a \) is equivalent to the norm induced by the inner product \( \langle -, - \rangle \) on \( V \). Thus \( h \) is still continuous with respect to the norm \( v \mapsto (a(v, v))^{1/2} \). Then by the Riesz representation theorem (Proposition 29.8), there is some unique \( c \in V \) such that
\[
h(v) = a(c, v) \quad \text{for all } v \in V.
\]
Consequently, we can express \( J(v) \) as
\[
J(v) = \frac{1}{2} a(v, v) - a(c, v) = \frac{1}{2} a(v - c, v - c) - \frac{1}{2} a(c, c).
\]
But then, minimizing \( J(v) \) over \( U \) is equivalent to minimizing \( (a(v - c, v - c))^{1/2} \) over \( v \in U \), and by the projection lemma (Proposition 29.5) this is equivalent to finding the projection \( p_U(c) \) of \( c \) on the closed convex set \( U \) with respect to the inner product \( a \). Therefore, there is a unique \( u = p_U(c) \in U \) such that
\[
J(u) = \inf_{v \in U} J(v).
\]
Also by Proposition 29.5, this unique element \( u \in U \) is characterized by the condition
\[
a(u - c, v - u) \geq 0 \quad \text{for all } v \in U.
\]
Since
\[
a(u - c, v - u) = a(u, v - u) - a(c, v - u) = a(u, v - u) - h(v - u),
\]
the above inequality is equivalent to
\[
a(u, v - u) \geq h(v - u) \quad \text{for all } v \in U. \quad (*)
\]
If \( U \) is a subspace of \( V \), then we have the condition
\[
a(u - c, v) = 0 \quad \text{for all } v \in U,
\]
which is equivalent to
\[
a(u, v) = a(c, v) = h(v) \quad \text{for all } v \in U. \quad (**)\]
Note that the symmetry of the bilinear form $a$ played a crucial role. Also, the inequalities

$$a(u, v - u) \geq h(v - u) \quad \text{for all } v \in U$$

are sometimes called \textit{variational inequalities}.

A bilinear form $a : V \times V \to \mathbb{R}$ such that there is some real $\alpha > 0$ such that

$$a(v, v) \geq \alpha \|v\|^2 \quad \text{for all } v \in V$$

is said to be \textit{coercive}.

Theorem 30.3 is the special case of Stampacchia’s theorem, and the Lax–Milgram theorem when $U = V$, in the case where $a$ is a symmetric bilinear form. To prove Stampacchia’s theorem in general, we need to recall the \textit{contraction mapping theorem}.

\textbf{Definition 13.4.} Let $(E, d)$ be a metric space. A map $f : E \to E$ is a \textit{contraction} (or a \textit{contraction mapping}) if there is some real number $k$ such that $0 \leq k < 1$ and

$$d(f(u), f(v)) \leq kd(u, v) \quad \text{for all } u, v \in E.$$ 

The number $k$ is often called a \textit{Lipschitz constant}.

The following theorem is proved in Section 19.8; see Theorem 19.23. A proof can be also found in Apostol [3], Dixmier [35], or Schwartz [91], among many sources. For the reader’s convenience we restate this theorem.

\textbf{Theorem 13.4.} (\textit{Contraction Mapping Theorem}) Let $(E, d)$ be a complete metric space. Every contraction $f : E \to E$ has a unique fixed point (that is, an element $u \in E$ such that $f(u) = u$).

The contraction mapping theorem is also known as the \textit{Banach fixed point theorem}.

\textbf{Theorem 13.5.} (Lions–Stampacchia) Given a Hilbert space $V$, let $a : V \times V \to \mathbb{R}$ be a continuous bilinear form (not necessarily symmetric), let $h \in V'$ be a continuous linear form, and let $J$ be given by

$$J(v) = \frac{1}{2} a(v, v) - h(v), \quad v \in V.$$ 

If $a$ is coercive, then for every nonempty, closed, convex subset $U$ of $V$, there is a unique $u \in U$ such that

$$a(u, v - u) \geq h(v - u) \quad \text{for all } v \in U. \quad (*)$$ 

If $a$ is symmetric, then $u \in U$ is the unique element of $U$ such that

$$J(u) = \inf_{v \in U} J(v).$$
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Proof. As discussed just after Definition 30.3, by Proposition 29.9, there is a unique continuous linear map $A : V \to V$ such that

$$a(u, v) = \langle Au, v \rangle \quad \text{for all } u, v \in V,$$

with $\|A\| = \|a\| = C$, and by the Riesz representation theorem (Proposition 29.8), there is a unique $b \in V$ such that

$$h(v) = \langle b, v \rangle \quad \text{for all } v \in V.$$

Consequently, $J$ can be written as

$$J(v) = \frac{1}{2} \langle Av, v \rangle - \langle b, v \rangle \quad \text{for all } v \in V. \quad (\ast_1)$$

Since $\|A\| = \|a\| = C$, we have $\|Av\| \leq \|A\| \|v\| = C \|v\|$ for all $v \in V$. Using $(\ast_1)$, the inequality $(\ast)$ is equivalent to finding $u$ such that

$$\langle Au, v - u \rangle \geq \langle b, v - u \rangle \quad \text{for all } v \in V. \quad (\ast_2)$$

Let $\rho > 0$ be a constant to be determined later. Then $(\ast_2)$ is equivalent to

$$\langle \rho b - \rho Au + u - u, v - u \rangle \leq 0 \quad \text{for all } v \in V. \quad (\ast_3)$$

By the projection lemma (Proposition 29.5), $(\ast_3)$ is equivalent to finding $u \in U$ such that

$$u = p_U(\rho b - \rho Au + u). \quad (\ast_4)$$

We are led to finding a fixed point of the function $F : V \to V$ given by

$$F(v) = p_U(\rho b - \rho Av + v).$$

By Proposition 29.6, the projection map $p_U$ does not increase distance, so

$$\|F(v_1) - F(v_2)\| \leq \|v_1 - v_2 - \rho(Av_1 - Av_2)\|.$$

Since $a$ is coercive we have

$$a(v, v) \geq \alpha \|v\|^2,$$

since $a(v, v) = \langle Av, v \rangle$ we have

$$\langle Av, v \rangle \geq \alpha \|v\|^2 \quad \text{for all } v \in V, \quad (\ast_5)$$

and since

$$\|Av\| \leq C \|v\| \quad \text{for all } v \in V, \quad (\ast_6)$$

we get

$$\|F(v_1) - F(v_2)\|^2 \leq \|v_1 - v_2\|^2 - 2\rho\langle Av_1 - Av_2, v_1 - v_2 \rangle + \rho^2 \|Av_1 - Av_2\|^2$$

$$\leq \left(1 - 2\rho \alpha + \rho^2 C\right) \|v_1 - v_2\|^2.$$
If we pick $\rho > 0$ such that $\rho < 2\alpha/C^2$, then

$$k^2 = 1 - 2\rho \alpha + \rho^2 C < 1,$$

and then

$$\|F(v_1) - F(v_2)\| \leq k \|v_1 - v_2\|,$$  \hspace{1cm} (*)

with $0 \leq k < 1$, which shows that $F$ is a contraction. By Theorem 30.4, the map $F$ has a unique fixed point $u \in U$, which concludes the proof of the first statement. If $a$ is also symmetric, then the second statement is just the first part of Proposition 30.3.

**Remark:** Many physical problems can be expressed in terms of an unknown function $u$ that satisfies some inequality

$$a(u, v - u) \geq h(v - u) \quad \text{for all } v \in U,$$

for some set $U$ of “admissible” functions which is closed and convex. The bilinear form $a$ and the linear form $h$ are often given in terms of integrals. The above inequality is called a *variational inequality*.

In the special case where $U = V$ we obtain the Lax–Milgram theorem.

**Theorem 13.6.** *(Lax–Milgram’s Theorem)* Given a Hilbert space $V$, let $a : V \times V \to \mathbb{R}$ be a continuous bilinear form (not necessarily symmetric), let $h \in V'$ be a continuous linear form, and let $J$ be given by

$$J(v) = \frac{1}{2} a(v, v) - h(v), \quad v \in V.$$  \hspace{1cm} \hspace{0.5cm} (1)

If $a$ is coercive, which means that there is some $\alpha > 0$ such that

$$a(v, v) \geq \alpha \|v\|^2 \quad \text{for all } v \in V,$$

then there is a unique $u \in V$ such that

$$a(u, v) = h(v) \quad \text{for all } v \in V.$$  \hspace{1cm} \hspace{0.5cm} (2)

If $a$ is symmetric, then $u \in V$ is the unique element of $V$ such that

$$J(u) = \inf_{v \in V} J(v).$$  \hspace{1cm} \hspace{0.5cm} (3)

The Lax–Milgram Theorem play an important role in solving linear elliptic partial differential equations; see Brezis [24].

We now consider various methods, known as gradient descents, to find minima of certain types of functionals.
13.2 Gradient Descent Methods for Unconstrained Problems

We begin by defining the notion of an elliptic functional which generalizes the notion of a quadratic function defined by a symmetric positive definite matrix. Elliptic functionals are well adapted to the types of iterative methods described in this section, and lend themselves well to an analysis of the convergence of these methods.

**Definition 13.5.** Given a Hilbert space $V$, a functional $J: V \to \mathbb{R}$ is said to be *elliptic* if it is continuously differentiable on $V$, and if there is some constant $\alpha > 0$ such that

$$\langle \nabla J_v - \nabla J_u, v - u \rangle \geq \alpha \|v - u\|^2 \quad \text{for all } u, v \in V.$$ 

The following proposition gathers properties of elliptic functionals that will be used later to analyze the convergence of various gradient descent methods.

**Theorem 13.7.** Let $V$ be a Hilbert space.

1. An elliptic functional $J: V \to \mathbb{R}$ is strictly convex and coercive. Furthermore, it satisfies the identity

   $$J(v) - J(u) \geq \langle \nabla J_u, v - u \rangle + \frac{\alpha}{2} \|v - u\|^2 \quad \text{for all } u, v \in V.$$ 

2. If $U$ is a nonempty, convex, closed subset of the Hilbert space $V$ and if $J$ is an elliptic functional, then the problem $(P)$,

   $$\text{find } u \quad \text{such that } u \in U \text{ and } J(u) = \inf_{v \in U} J(v)$$

   has a unique solution.

3. Suppose the set $U$ is convex and that the functional $J$ is elliptic. Then an element $u \in U$ is a solution of the problem $(P)$ if and only if it satisfies the condition

   $$\langle \nabla J_u, v - u \rangle \geq 0 \quad \text{for every } v \in U$$

   in the general case, or

   $$\nabla J_u = 0 \quad \text{if } U = V$$

4. A functional $J$ which is twice differentiable in $V$ is elliptic if and only if

   $$\langle \nabla^2 J_u(w), w \rangle \geq \alpha \|w\|^2 \quad \text{for all } u, w \in V.$$
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Proof. (1) Since \( J \) is a \( C^1 \)-function, by Taylor’s formula with integral remainder in the case \( m = 0 \) (Theorem 20.24), we get

\[
J(v) - J(u) = \int_0^1 dJ_{u+t(v-u)}(v-u)dt
\]

\[
= \int_0^1 \langle \nabla J_{u+t(v-u)}, v-u \rangle dt
\]

\[
= \langle \nabla J_u, v-u \rangle + \int_0^1 \langle \nabla J_{u+t(v-u)} - \nabla J_u, t(v-u) \rangle dt
\]

\[
\geq \langle \nabla J_u, v-u \rangle + \int_0^1 \alpha t \|v-u\|^2 dt \quad \text{since } J \text{ is elliptic}
\]

\[
= \langle \nabla J_u, v-u \rangle + \frac{\alpha}{2} \|v-u\|^2.
\]

Using the inequality

\[
J(v) - J(u) \geq \langle \nabla J_u, v-u \rangle + \frac{\alpha}{2} \|v-u\|^2 \quad \text{for all } u,v \in V,
\]

by Proposition 21.9(2), since

\[
J(v) > J(u) + \langle \nabla J_u, v-u \rangle \quad \text{for all } u,v \in V, \ v \neq u,
\]

the function \( J \) is strictly convex. It is coercive because

\[
J(v) \geq J(0) + \langle \nabla J_0, v \rangle + \frac{\alpha}{2} \|v\|^2
\]

\[
\geq J(0) - \|\nabla J_0\| \|v\| + \frac{\alpha}{2} \|v\|^2,
\]

and the term \((- \|\nabla J_0\| + \frac{\alpha}{2} \|v\|) \|v\|\) goes to \(+\infty\) when \(\|v\|\) tends to \(+\infty\).

(2) Since by (1) the functional \( J \) is coercive, by Theorem 30.2, problem (P) has a solution. Since \( J \) is strictly convex, by Theorem 21.11(2), it has a unique minimum.

(3) These are just the conditions of Theorem 21.11(3, 4).

(4) If \( J \) is twice differentiable, we showed in Section 20.4 that we have

\[
D^2 J_u(w,w) = D_u(DJ)(u) = \lim_{\theta \to 0} \frac{DJ_{u+\theta w}(w) - DJ_u(w)}{\theta},
\]

and since

\[
D^2 J_u(w,w) = \langle \nabla^2 J_u(w), w \rangle
\]

\[
DJ_{u+\theta w}(w) = \langle \nabla J_{u+\theta w}, w \rangle
\]

\[
DJ_u(w) = \langle \nabla J_u, w \rangle,
\]
and since $J$ is elliptic, for all $u, w \in V$ we can write

$$
\langle \nabla^2 J_u(w), w \rangle = \lim_{\theta \to 0} \frac{\langle \nabla J_{u+\theta w} - \nabla J_u, w \rangle}{\theta}
= \lim_{\theta \to 0} \frac{\langle \nabla J_{u+\theta w} - \nabla J_u, \theta w \rangle}{\theta^2}
\geq \alpha \|w\|^2.
$$

Conversely, assume that the condition

$$
\langle \nabla^2 J_u(w), w \rangle \geq \alpha \|w\|^2 \quad \text{for all } u, w \in V
$$

holds. If we define the function $g: V \to \mathbb{R}$ by

$$
g(w) = \langle \nabla J_w, v - u \rangle = dJ_w(v - u) = D_{v-u}J(w),
$$

where $u$ and $v$ are fixed vectors in $V$, then we have

$$
dg_{u+\theta(v-u)}(v-u) = D_{v-u}g(u+\theta(v-u)) = D_{v-u}D_{v-u}J(u+\theta(v-u)) = D^2 J_{u+\theta(v-u)}(v-u, v-u)
$$

and we can apply the Taylor–MacLaurin formula (Theorem 20.23 with $m = 0$) to $g$, and we get

$$
\langle \nabla J_v - \nabla J_u, v - u \rangle
= g(v) - g(u)
= dg_{u+\theta(v-u)}(v-u) \quad (0 < \theta < 1)
= D^2 J_{u+\theta(v-u)}(v-u, v-u)
= \langle \nabla^2 J_{u+\theta(v-u)}(v-u), v - u \rangle
\geq \alpha \|v - u\|^2,
$$

which shows that $J$ is elliptic. \qed

If $J: \mathbb{R}^n \to \mathbb{R}$ is a quadratic function given by

$$
J(v) = \frac{1}{2} \langle Av, v \rangle - \langle b, v \rangle
$$

(where $A$ is a symmetric $n \times n$ matrix and $\langle -, - \rangle$ is the standard Euclidean inner product), then $J$ is elliptic iff $A$ is positive definite. This is because

$$
\langle \nabla^2 J_u(w), w \rangle = \langle Aw, w \rangle \geq \lambda_1 \|w\|^2
$$

where $\lambda_1$ is the smallest eigenvalue of $A$; see Proposition 14.23 (Rayleigh–Ritz, Vol. I). Note that by Proposition 14.23 (Rayleigh–Ritz, Vol. I), we also have

$$
\langle \nabla^2 J_u(w), w \rangle \leq \lambda_n \|w\|^2
$$
where $\lambda_n$ is the largest eigenvalue of $A$; this fact will be useful later on.

Similarly, given a quadratic functional $J$ defined on a Hilbert space $V$, where

$$J(v) = \frac{1}{2}a(v, v) - h(v),$$

by Theorem 30.7 (4), the functional $J$ is elliptic iff there is some $\alpha > 0$ such that

$$\langle \nabla^2 J_u(v), v \rangle = a(v, v) \geq \alpha \|v\|^2 \quad \text{for all } v \in V.$$

This is precisely the hypothesis ($*_\alpha$) used in Theorem 30.3.

We will now describe methods for solving unconstrained minimization problems, that is, finding the minimum (or minima) of a function $J$ over the whole space $V$. These methods are iterative, which means that given some initial vector $u_0$, we construct a sequence $(u_k)_{k \geq 0}$ that converges to a minimum $u$ of the function $J$.

The key step is define $u_{k+1}$ from $u_k$, and a first idea is to reduce the problem to a simpler problem, namely the minimization of a function of a single (real) variable. For this, we need two perform two steps:

1. Find a **descent direction** at $u_k$, which is a some nonzero vector $d_k$ which is usually determined from the gradient of $J$ at various points.

2. Find the minimum of the restriction of the function $J$ along the line through $u_k$ and parallel to the direction $d_k$. This means finding a real $\rho_k \in \mathbb{R}$ (depending on $u_k$ and $d_k$) such that

$$J(u_k + \rho_k d_k) = \inf_{\rho \in \mathbb{R}} J(u_k + \rho d_k).$$

This problem only succeeds if $\rho_k$ is unique, in which case we set

$$u_{k+1} = u_k + \rho_k d_k.$$

This step is often called a **line search** or **line minimization**, and $\rho_k$ is called the **stepsize** parameter. See Figure 30.1.

If $J$ is a quadratic elliptic functional of the form

$$J(v) = \frac{1}{2}a(v, v) - h(v),$$

then given $d_k$, there is a unique $\rho_k$ solving the line search in Step (2). This is because, as we explained earlier, we have

$$J(u_k + \rho d_k) = \frac{\rho^2}{2}a(d_k, d_k) + \rho \langle \nabla J_{u_k}, d_k \rangle + J(u_k),$$
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\[ J(u_{k+1}) = \inf_{\lambda \in \mathbb{R}} J(\lambda, u_{k+1}^{k+1}) \]

\[ J(u_{k+1}^{k+1}) = \inf_{\lambda \in \mathbb{R}} J(u_{k+1}^{k+1}, \lambda) \]

Another and more informative way to write the above system is to define the vectors \( u_{k:i} \)

Figure 13.1: Let \( J : \mathbb{R}^2 \to \mathbb{R} \) be the function whose graph is represented by the pink surface. Given a point \( u_k \) in the \( xy \)-plane, and a direction \( d_k \), we calculate first \( u_{k+1} \) and then \( u_{k+2} \).

and since \( a(d_k, d_k) > 0 \) (because \( J \) is elliptic), the above function of \( \rho \) has a unique minimum when its derivative is zero, namely

\[ \rho a(d_k, d_k) + \langle \nabla J_{u_k}, d_k \rangle = 0. \]

We now consider one of the simplest methods for choosing the directions of descent in the case where \( V = \mathbb{R}^n \), which is to pick the directions of the coordinate axes in a cyclic fashion. Such a method is called the method of relaxation.

If we write

\[ u_k = (u_k^1, u_k^2, \ldots, u_k^n), \]

then the components \( u_{k+1}^{k+1} \) of \( u_{k+1} \) are computed in terms of \( u_k \) by solving from top down the following system of equations:

\[ J(u_{k+1}^{k+1}, u_2^1, u_3^1, \ldots, u_n^1) = \inf_{\lambda \in \mathbb{R}} J(\lambda, u_2^1, u_3^1, \ldots, u_n^1) \]

\[ J(u_{k+1}^{k+1}, u_{k+1}^{k+1}, u_3^1, \ldots, u_n^1) = \inf_{\lambda \in \mathbb{R}} J(u_{k+1}^{k+1}, \lambda, u_3^1, \ldots, u_n^1) \]

\[ \vdots \]

\[ J(u_{k+1}^{k+1}, \ldots, u_{k+1}^{k+1}, u_{k+1}^{k+1}) = \inf_{\lambda \in \mathbb{R}} J(u_{k+1}^{k+1}, \ldots, u_{k+1}^{k+1}, \lambda). \]
by

\[ u_{k;0} = (u_1^k, u_2^k, \ldots, u_n^k) \]
\[ u_{k;1} = (u_1^{k+1}, u_2^k, \ldots, u_n^k) \]
\[ \vdots \]
\[ u_{k;i} = (u_1^{k+1}, \ldots, u_i^{k+1}, u_{i+1}^k, \ldots, u_n^k) \]
\[ \vdots \]
\[ u_{k;n} = (u_1^{k+1}, u_2^{k+1}, \ldots, u_n^{k+1}). \]

Note that \( u_{k;0} = u_k \) and \( u_{k;n} = u_{k+1} \). Then our minimization problem can be written as

\[ J(u_{k;1}) = \inf_{\lambda \in \mathbb{R}} J(u_{k;0} + \lambda e_1) \]
\[ \vdots \]
\[ J(u_{k;i}) = \inf_{\lambda \in \mathbb{R}} J(u_{k;i-1} + \lambda e_i) \]
\[ \vdots \]
\[ J(u_{k;n}) = \inf_{\lambda \in \mathbb{R}} J(u_{k;n-1} + \lambda e_n), \]

where \( e_i \) denotes the \( i \)th canonical basis vector in \( \mathbb{R}^n \). If \( J \) is differentiable, necessary conditions for a minimum, which are also sufficient if \( J \) is convex, is that the directional derivatives \( dJ_u(e_i) \) be all zero, that is,

\[ \langle \nabla J_u, e_i \rangle = 0 \quad i = 0, \ldots, n. \]

The following result regarding the convergence of the method of relaxation is proved in Ciarlet [30] (Chapter 8, Theorem 8.4.2).

**Proposition 13.8.** If the functional \( J: \mathbb{R}^n \rightarrow \mathbb{R} \) is elliptic, then the relaxation method converges.

**Remarks:** The proof of Proposition 30.8 uses Theorem 30.7. The finite dimensionality of \( \mathbb{R}^n \) also plays a crucial role. The differentiability of the function \( J \) is also crucial. Examples where the method loops forever if \( J \) is not differentiable can be given; see Ciarlet [30] (Chapter 8, Section 8.4). The proof of Proposition 30.8 yields an *a priori* bound on the error \( \| u - u_k \| \). If \( J \) is a quadratic functional

\[ J(v) = \frac{1}{2} v^\top A v - b^\top v, \]

where \( A \) is a symmetric positive definite matrix, then \( \nabla J_v = Av - b \), so the above system to solve for \( u_{k+1} \) in terms of \( u_k \) becomes the *Gauss-Seidel method* for solving a linear system; see Section 8.3 (Vol. I).
We now discuss gradient methods. The intuition behind these methods is that the convergence of an iterative method ought to be better if the difference $J(u_k) - J(u_{k+1})$ is as large as possible during every iteration step. To achieve this, it is natural to pick the descent direction to be the one in the opposite direction of the gradient vector $\nabla J_{u_k}$. This choice is justified by the fact that we can write

$$J(u_k + w) = J(u_k) + \langle \nabla J_{u_k}, w \rangle + \epsilon(w) \|w\|,$$

with $\lim_{w \to 0} \epsilon(w) = 0$.

If $\nabla J_{u_k} \neq 0$, the first-order part of the variation of the function $J$ is bounded in absolute value by $\|\nabla J_{u_k}\| \|w\|$ (by the Cauchy–Schwarz inequality), with equality if $\nabla J_{u_k}$ and $w$ are collinear.

Gradient descent methods pick the direction of descent to be $d_k = -\nabla J_{u_k}$, so that we have

$$u_{k+1} = u_k - \rho_k \nabla J_{u_k},$$

where we put a negative sign in front of of the variable $\rho_k$ as a reminder that the descent direction is opposite to that of the gradient; a positive value is expected for the scalar $\rho_k$.

There are three standard methods to pick $\rho_k$:

1. **Gradient method with fixed stepsize parameter.** This is the simplest and cheapest method which consists of using the same constant $\rho_k = \rho$ for all iterations.

2. **Gradient method with variable stepsize parameter.** In this method, the parameter $\rho_k$ is adjusted in the course of iterations according to various criteria.

3. **Gradient method with optimal stepsize parameter**, also called steepest descent method for the Euclidean norm. This is a version of method 2 in which $\rho_k$ is determined by the following line search:

$$J(u_k - \rho_k \nabla J_{u_k}) = \inf_{\rho \in \mathbb{R}} J(u_k - \rho \nabla J_{u_k}).$$

This optimization problem only succeeds if the above minimization problem has a unique solution.

We have the following useful result about the convergence of the gradient method with optimal parameter.

**Proposition 13.9.** Let $J : \mathbb{R}^n \to \mathbb{R}$ be an elliptic functional. Then the gradient method with optimal stepsize parameter converges.

**Proof.** Since $J$ is elliptic, by Theorem 30.7, the functional $J$ has a unique minimum $u$ characterized by $\nabla J_u = 0$. Our goal is to prove that the sequence $(u_k)_{k \geq 0}$ constructed using the gradient method with optimal parameter converges to $u$, started from any initial vector $u_0$. Without loss of generality we may assume that $u_{k+1} \neq u_k$ and $\nabla J_{u_k} \neq 0$ for all $k$, since otherwise the method converges in a finite number of steps.
**Step 1.** Any two consecutive descent directions are orthogonal, and
\[ J(u_k) - J(u_{k+1}) \geq \frac{\alpha}{2} \| u_k - u_{k+1} \|^2. \]

Let \( \varphi_k : \mathbb{R} \to \mathbb{R} \) be the function given by
\[ \varphi_k(\rho) = J(u_k - \rho \nabla J_{u_k}). \]

Since the function \( \varphi_k \) is strictly convex and coercive, it has a unique minimum \( \rho_k \) which is the unique solution of the equation \( \varphi'_k(\rho) = 0 \). By the chain rule
\[ \varphi'_k(\rho) = dJ_{u_k - \rho \nabla J_{u_k}} (-\nabla J_{u_k}) \]
\[ = -\langle \nabla J_{u_k - \rho \nabla J_{u_k}}, \nabla J_{u_k} \rangle, \]
and since \( u_{k+1} = u_k - \rho_k \nabla J_{u_k} \) we get
\[ \langle \nabla J_{u_{k+1}}, \nabla J_{u_k} \rangle = 0, \]
which shows that two consecutive descent directions are orthogonal.

Since \( u_{k+1} = u_k - \rho_k \nabla J_{u_k} \) and we assumed that that \( u_{k+1} \neq u_k \), we have \( \rho_k \neq 0 \), and we also get
\[ \langle \nabla J_{u_{k+1}}, u_{k+1} - u_k \rangle = 0. \]

By the inequality of Theorem 30.7(1) we have
\[ J(u_k) - J(u_{k+1}) \geq \frac{\alpha}{2} \| u_k - u_{k+1} \|^2. \]

**Step 2.** \( \lim_{k \to \infty} \| u_k - u_{k+1} \| = 0. \)

It follows from the inequality proved in Step 1 that the sequence \((J(u_k))_{k \geq 0}\) is decreasing and bounded below (by \( J(u) \), where \( u \) is the minimum of \( J \)), so it converges and we conclude that
\[ \lim_{k \to \infty} (J(u_k) - J(u_{k+1})) = 0, \]
which combined with the preceding inequality shows that
\[ \lim_{k \to \infty} \| u_k - u_{k+1} \| = 0. \]

**Step 3.** \( \| \nabla J_{u_k} \| \leq \| \nabla J_{u_k} - \nabla J_{u_{k+1}} \|. \)

Using the orthogonality of consecutive descent directions, by Cauchy–Schwarz we have
\[ \| \nabla J_{u_k} \|^2 = \langle \nabla J_{u_k}, \nabla J_{u_k} - \nabla J_{u_{k+1}} \rangle \]
\[ \leq \| \nabla J_{u_k} \| \| \nabla J_{u_k} - \nabla J_{u_{k+1}} \|. \]
so that
\[ \| \nabla J_{u_k} \| \leq \| \nabla J_{u_k} - \nabla J_{u_{k+1}} \|. \]

**Step 4.** \( \lim_{k \to \infty} \| \nabla J_{u_k} \| = 0. \)

Since the sequence \((J(u_k))_{k \geq 0}\) is decreasing and the functional \(J\) is coercive, the sequence \((u_k)_{k \geq 0}\) must be bounded. By hypothesis, the derivative \(dJ\) is of \(J\) is continuous, so it is uniformly continuous over compact subsets of \(\mathbb{R}^n\); here, we are using the fact that \(\mathbb{R}^n\) is finite dimensional. Hence, we deduce that for every \(\epsilon > 0\), if \(\| u_k - u_{k+1} \| < \epsilon \) then
\[ \| dJ_{u_k} - dJ_{u_{k+1}} \|_2 < \epsilon. \]

But by definition of the operator norm and using the Cauchy–Schwarz inequality
\[ \| dJ_{u_k} - dJ_{u_{k+1}} \|_2 = \sup_{\| w \| \leq 1} | dJ_{u_k}(w) - dJ_{u_{k+1}}(w) | \]
\[ = \sup_{\| w \| \leq 1} | \langle \nabla J_{u_k} - \nabla J_{u_{k+1}}, w \rangle | \]
\[ \leq \| \nabla J_{u_k} - \nabla J_{u_{k+1}} \|. \]

But we also have
\[ \| \nabla J_{u_k} - \nabla J_{u_{k+1}} \|^2 = \langle \nabla J_{u_k} - \nabla J_{u_{k+1}}, \nabla J_{u_k} - \nabla J_{u_{k+1}} \rangle \]
\[ = \langle \nabla J_{u_k} - \nabla J_{u_{k+1}} \rangle \]
\[ \leq \| dJ_{u_k} - dJ_{u_{k+1}} \|_2^2, \]

and so
\[ \| dJ_{u_k} - dJ_{u_{k+1}} \|_2 = \| \nabla J_{u_k} - \nabla J_{u_{k+1}} \|. \]

It follows that if
\[ \lim_{k \to \infty} \| u_k - u_{k+1} \| = 0 \]
then
\[ \lim_{k \to \infty} \| \nabla J_{u_k} - \nabla J_{u_{k+1}} \| = \lim_{k \to \infty} \| dJ_{u_k} - dJ_{u_{k+1}} \|_2 = 0, \]

and using the fact that
\[ \| \nabla J_{u_k} \| \leq \| \nabla J_{u_k} - \nabla J_{u_{k+1}} \|, \]

we obtain
\[ \lim_{k \to \infty} \| \nabla J_{u_k} \| = 0. \]

**Step 5.** Finally we can prove the convergence of the sequence \((u_k)_{k \geq 0}\).

Since \(J\) is elliptic and since \(\nabla J_u = 0\) (since \(u\) is the minimum of \(J\) over \(\mathbb{R}^n\)), we have
\[ \alpha \| u_k - u \|^2 \leq \langle \nabla J_{u_k} - \nabla J_u, u_k - u \rangle \]
\[ = \langle \nabla J_{u_k}, u_k - u \rangle \]
\[ \leq \| \nabla J_{u_k} \| \| u_k - u \|. \]
Hence, we obtain
\[ \|u_k - u\| \leq \frac{1}{\alpha} \|\nabla J_{u_k}\|, \]
and since we showed that
\[ \lim_{k \to \infty} \|\nabla J_{u_k}\| = 0, \]
we see that the sequence \((u_k)_{k \geq 0}\) converges to the minimum \(u\).

**Remarks:** As with the previous proposition, the assumption of finite dimensionality is crucial. The proof provides an *a priori* bound on the error \(\|u_k - u\|\).

If \(J\) is a an elliptic quadratic functional
\[ J(v) = \frac{1}{2} \langle Av, v \rangle - \langle b, v \rangle, \]
we can use the orthogonality of the descent directions \(\nabla J_{u_k}\) and \(\nabla J_{u_{k+1}}\) to compute \(\rho_k\). Indeed, we have \(\nabla J_v = Av - b\), so
\[ 0 = \langle \nabla J_{u_{k+1}}, \nabla J_{u_k} \rangle = \langle A(u_k - \rho_k(Au_k - b)) - b, Au_k - b \rangle, \]
which yields
\[ \rho_k = \frac{\|w_k\|^2}{\langle Aw_k, w_k \rangle}, \quad \text{with} \quad w_k = Au_k - b = \nabla J_{u_k}. \]

Consequently, a step of the iteration method takes the following form:

1. Compute the vector
   \[ w_k = Au_k - b. \]
2. Compute the scalar
   \[ \rho_k = \frac{\|w_k\|^2}{\langle Aw_k, w_k \rangle}. \]
3. Compute the next vector \(u_{k+1}\) by
   \[ u_{k+1} = u_k - \rho_k w_k. \]

This method is of particular interest when the computation of \(Aw\) for a given vector \(w\) is cheap, which is the case if \(A\) is sparse.

For a particular illustration of this method, we turn to the example provided by Shewchuk, with \(A = \begin{pmatrix} 3 & 2 \\ 2 & 6 \end{pmatrix}\) and \(b = \begin{pmatrix} 2 \\ -8 \end{pmatrix}\), namely
\[ J(x, y) = \frac{1}{2} \begin{pmatrix} x & y \end{pmatrix} \begin{pmatrix} 3 & 2 \\ 2 & 6 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} - (2 - 8) \begin{pmatrix} x \\ y \end{pmatrix} \]
\[ = \frac{3}{2} x^2 + 2xy + 3y^2 - 2x + 8y. \]
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Figure 13.2: The ellipsoid $J(x, y) = \frac{3}{2}x^2 + 2xy + 3y^2 - 2x + 8y$.

This quadratic ellipsoid, which is illustrated in Figure 30.2, has a unique minimum at $(2, -2)$. In order to find this minimum via the gradient descent with optimal step size parameter, we pick a starting point, say $u_k = (-2, -2)$, and calculate the search direction $w_k = \nabla J(-2, -2) = (-12, -8)$. Note that

$$\nabla J(x, y) = (3x + 2y - 2, 2x + 6y + 8) = \begin{pmatrix} 3 & 2 \\ 2 & 6 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} - \begin{pmatrix} 2 \\ 8 \end{pmatrix}$$

is perpendicular to the appropriate elliptical level curve; see Figure 30.3. We next perform

Figure 13.3: The level curves of $J(x, y) = \frac{3}{2}x^2 + 2xy + 3y^2 - 2x + 8y$ and the associated gradient vector field $\nabla J(x, y) = (3x + 2y - 2, 2x + 6y + 8)$.

the line search along the line given by the equation $-8x + 12y = -8$ and determine $\rho_k$. See Figures 30.4 and 30.5. In particular, we find that
Figure 13.4: The level curves of \( J(x, y) = \frac{3}{2}x^2 + 2xy + 3y^2 - 2x + 8y \) and the red search line with direction \( \nabla J(-2, -2) = (-12, -8) \)

\[
\rho_k = \frac{\|w_k\|^2}{\langle Aw_k, w_k \rangle} = \frac{13}{75}.
\]

This in turn gives us the new point
\[
u_{k+1} = u_k - \frac{13}{75} w_k = (-2, -2) - \frac{13}{75}(-12, -8) = \left( \frac{2}{25}, -\frac{46}{75} \right),
\]

and we continue the procedure by searching along the gradient direction \( \nabla J(2/25, -46/75) = (-224/75, 112/25) \). Observe that \( u_{k+1} = \left( \frac{2}{25}, -\frac{46}{75} \right) \) has a gradient vector which is perpendicular to the search line with direction vector \( w_k = \nabla J(-2, -2) = (-12, -8) \); see Figure 30.5. Geometrically this procedure corresponds to intersecting the plane \(-8x + 2y = -8\) with the ellipsoid \( J(x, y) = \frac{3}{2}x^2 + 2xy + 3y^2 - 2x + 8y \) to form the parabolic curve \( f(x) = \frac{25}{6}x^2 - 3x - 4 \) and then locating the \( x \)-coordinate of its apex which occurs when \( f'(x) = 0 \), i.e when \( x = 2/25 \); see Figure 30.6. After 31 iterations, this procedure stabilizes to point \((2, -2)\), which as we know, is the unique minimum of the quadratic ellipsoid \( J(x, y) = \frac{3}{2}x^2 + 2xy + 3y^2 - 2x + 8y \).

We now give a sufficient condition for the gradient method with variable stepsize parameter to converge. In addition to requiring \( J \) to be an elliptic functional, we add a Lipschitz condition on the gradient of \( J \). This time, the space \( V \) can be infinite dimensional.

**Proposition 13.10.** Let \( J: V \to \mathbb{R} \) be a continuously differentiable functional defined on a Hilbert space \( V \). Suppose there exists two constants \( \alpha > 0 \) and \( M > 0 \) such that
\[
\langle \nabla J_v - \nabla J_u, v - u \rangle \geq \alpha \|v - u\|^2 \quad \text{for all } u, v \in V,
\]
and
\[
\|\nabla J_v - \nabla J_u\| \leq M \|v - u\| \quad \text{for all } u, v \in V.
\]
If there exists two real numbers $a, b \in \mathbb{R}$ such that

$$0 < a \leq \rho_k \leq b \leq \frac{2\alpha}{M^2} \quad \text{for all } k \geq 0,$$

then the gradient method with variable stepsize parameter converges. Furthermore, there is some constant $\beta > 0$ (depending on $\alpha, M, a, b$) such that

$$\beta < 1 \quad \text{and} \quad \|u_k - u\| \leq \beta^k \|u_0 - u\|,$$

where $u \in M$ is the unique minimum of $J$.

Proof. By hypothesis the functional $J$ is elliptic, so by Theorem 30.7 it has a unique minimum $u$ characterized by the fact that $\nabla J_u = 0$. Then since $u_{k+1} = u_k - \rho_k \nabla J_{u_k}$ we can write

$$u_{k+1} - u = (u_k - u) - \rho_k \langle \nabla J_{u_k} - \nabla J_u \rangle.$$

Using the inequalities

$$\langle \nabla J_{u_k} - \nabla J_u, u_k - u \rangle \geq \alpha \|u_k - u\|^2$$

and

$$\|\nabla J_{u_k} - \nabla J_u\| \leq M \|u_k - u\|,$$

and assuming that $\rho_k > 0$, it follows that

$$\|u_{k+1} - u\|^2 = \|u_k - u\|^2 - 2\rho_k \langle \nabla J_{u_k} - \nabla J_u, u_k - u \rangle + \rho_k^2 \|\nabla J_{u_k} - \nabla J_u\|^2$$

$$\leq \left(1 - 2\alpha \rho_k + M^2 \rho_k^2\right) \|u_k - u\|^2.$$
## CHAPTER 13. GENERAL RESULTS OF OPTIMIZATION THEORY

Figure 13.6: Two views of the intersection between the plane $-8x + 12y = -8$ and the ellipsoid $J(x, y) = \frac{3}{2}x^2 + 2xy + 3y^2 - 2x + 8y$. The point $u_{k+1}$ is the minimum of the parabolic intersection.

Consider the function

$$T(\rho) = M^2 \rho^2 - 2\alpha \rho + 1.$$  

Its graph is a parabola intersecting the $y$-axis at $y = 1$ for $\rho = 0$, it has a minimum for $\rho = \alpha/M^2$, and it also has the value $y = 1$ for $\rho = 2\alpha/M^2$; see Figure 30.7. Therefore if we pick $a, b$ and $\rho_k$ such that

$$0 < a \leq \rho_k \leq b < \frac{2\alpha}{M^2},$$

we ensure that for $\rho \in [a, b]$ we have

$$T(\rho)^{1/2} = (M^2 \rho^2 - 2\alpha \rho + 1)^{1/2} \leq (\max\{T(a), T(b)\})^{1/2} = \beta < 1.$$  

Then by induction we get

$$\|u_{k+1} - u\| \leq \beta^{k+1} \|u_0 - u\|,$$

which proves convergence.

\[\square\]

**Remarks:** In the proof of Proposition 30.10, it is the fact that $V$ is complete which plays a crucial role. If $J$ is twice differentiable, the hypothesis

$$\|\nabla J_v - \nabla J_u\| \leq M \|v - u\| \quad \text{for all } u, v \in V$$

would
can be expressed as

$$\sup_{v \in V} \left\| \nabla^2 J_v \right\| \leq M.$$ 

In the case of a quadratic elliptic functional defined over $\mathbb{R}^n$,

$$J(v) = \langle Av, v \rangle - \langle b, v \rangle,$$

the upper bound $2\alpha/M^2$ can be improved. In this case we have

$$\nabla J_v = Av - b,$$

and we know that we $\alpha = \lambda_1$ and $M = \lambda_n$ do the job, where $\lambda_1$ is the eigenvalue of $A$ and $\lambda_n$ is the largest eigenvalue of $A$. Hence we can pick $a, b$ such that

$$0 < a \leq \rho_k \leq b < \frac{2\lambda_1}{\lambda_n^2}.$$ 

Since $u_{k+1} = u_k - \rho_k \nabla J_{u_k}$ and $\nabla J_{u_k} = Au_k - b$, we have

$$u_{k+1} - u = (u_k - u) - \rho_k (Au_k - u) = (I - \rho_k A)(u_k - u),$$

so we get

$$\|u_{k+1} - u\| \leq \|I - \rho_k A\|_2 \|u_k - u\|.$$ 

However, since $I - \rho_k A$ is a symmetric matrix, $\|I - \rho_k A\|_2$ is the largest absolute value of its eigenvalues, so

$$\|I - \rho_k A\|_2 \leq \max\{\|1 - \rho_k \lambda_1\|, \|1 - \rho_k \lambda_n\|\}.$$ 

The function

$$\mu(\rho) = \max\{\|1 - \rho \lambda_1\|, \|1 - \rho \lambda_n\|\}$$

is a piecewise affine function, and it is easy to see that if we pick $a, b$ such that

$$0 < a \leq \rho_k \leq b \leq \frac{2}{\lambda_n},$$
then
\[
\max_{\rho \in [a, b]} \mu(\rho) \leq \max\{\mu(a), \mu(b)\} < 1.
\]

Therefore, the upper bound \(2\lambda_1/\lambda_n^2\) can be replaced by \(2/\lambda_n\), which is typically much larger. A “good” pick for \(\rho_k\) is \(2/(\lambda_1 + \lambda_n)\) (as opposed to \(\lambda_1/\lambda_n^2\) for the first version). In this case
\[
|1 - \rho_k\lambda_1| = |1 - \rho_k\lambda_n| = \frac{\lambda_m - \lambda_1}{\lambda_m + \lambda_1},
\]
so we get
\[
\beta = \frac{\lambda_m - \lambda_1}{\lambda_m + \lambda_1} = \frac{\frac{\lambda_m}{\lambda_1} - 1}{\frac{\lambda_m}{\lambda_1} + 1} = \frac{\text{cond}_2(A) - 1}{\text{cond}_2(A) + 1},
\]
where \(\text{cond}_2(A) = \lambda_m/\lambda_1\) is the condition number of the matrix \(A\) with respect to the spectral norm. Thus we see that the largest the condition number of \(A\) is, the slowest the convergence of the method will be. This is not surprising since we already know that linear systems involving ill-conditioned matrices (matrices with a large condition number) are problematic, and prone to numerical unstability. One way to deal with this problem is to use a method known as preconditioning.

We only described the most basic gradient descent methods. There are numerous variants, and we only mention a few of these methods.

The method of scaling consists in using \(-\rho_kD_k\nabla J_{u_k}\) as descent direction, where \(D_k\) is some suitably chosen symmetric positive definite matrix.

In the gradient method with extrapolation, \(u_{k+1}\) is determined by
\[
u_{k+1} = u_k - \rho_k\nabla J_{u_k} + \beta_k(u_k - u_{k-1}).
\]

Another rule for choosing the stepsize is Armijo’s rule.

These methods, and others, are discussed in detail in Berstekas [14]. Boyd and Vandenberghe discuss steepest descent methods for various types of norms besides the Euclidean norm; see Boyd and Vandenberghe [22] (Section 9.4).

Lax also discusses other methods in which the step \(\rho_k\) is chosen using roots of Chebyshev polynomials; see Lax [67], Chapter 17, Sections 2–4.

Contrary to intuition, the descent direction \(d_k = -\nabla J_{u_k}\) given by the opposite of the gradient is not optimal. In the next section, we will see how a better direction can be picked; this is the method of conjugate gradients.
13.3 Conjugate Gradient Methods for Unconstrained Problems

The conjugate gradient method due to Hestenes and Stiefel (1952) is a gradient descent method that applies to an elliptic quadratic functional $J: \mathbb{R}^n \to \mathbb{R}$ given by

$$J(v) = \frac{1}{2} \langle Av, v \rangle - \langle b, v \rangle,$$

where $A$ is an $n \times n$ symmetric positive definite matrix. Although it is presented as an iterative method, it terminates in at most $n$ steps.

As usual, the conjugate gradient method starts with some arbitrary initial vector $u_0$ and proceeds through a sequence of iteration steps generating (better and better) approximations $u_k$ of the optimal vector $u$ minimizing $J$. During an iteration step, two vectors need to be determined:

1. The descent direction $d_k$.
2. The next approximation $u_{k+1}$. To find $u_{k+1}$, we need to find the stepsize $\rho_k > 0$ and then

$$u_{k+1} = u_k - \rho_k d_k.$$

Typically, $\rho_k$ is found by performing a line search along the direction $d_k$, namely we find $\rho_k$ as the real number such that the function $\rho \mapsto J(u_k - \rho d_k)$ is minimized.

We saw in Proposition 30.9 that during execution of the gradient method with optimal stepsize parameter that any two consecutive descent directions are orthogonal. The new twist with the conjugate gradient method is that given $u_0, u_1, \ldots, u_k$, the next approximation $u_{k+1}$ is obtained as the solution of the problem which consists in minimizing $J$ over the affine subspace $u_k + G_k$, where $G_k$ is the subspace of $\mathbb{R}^n$ spanned by the gradients

$$\nabla J_{u_0}, \nabla J_{u_1}, \ldots, \nabla J_{u_k}.$$

We may assume that $\nabla J_{u_\ell} \neq 0$ for $\ell = 0, \ldots, k$, since the method terminates as soon as $\nabla J_{u_k} = 0$. A priori the subspace $G_k$ has dimension $\leq k + 1$, but we will see that in fact it has dimension $k + 1$. Then we have

$$u_k + G_k = \left\{ u_k + \sum_{i=0}^k \alpha_i \nabla J_{u_i} \mid \alpha_i \in \mathbb{R}, \ 0 \leq i \leq k \right\},$$

and our minimization problem is to find $u_{k+1}$ such that

$$u_{k+1} \in u_k + G_k \quad \text{and} \quad J(u_{k+1}) = \inf_{v \in u_k + G_k} J(v).$$
In the gradient method with optimal stepsize parameter the descent direction \( d_k \) is proportional to the gradient \( \nabla J_{u_k} \), but in the conjugate gradient method, \( d_k \) is equal to \( \nabla J_{u_k} \) corrected by some multiple of \( d_{k-1} \).

The conjugate gradient method is superior to the gradient method with optimal stepsize parameter for the following reasons proved correct later:

(a) The gradients \( \nabla J_{u_i} \) and \( \nabla J_{u_j} \) are orthogonal for all \( i, j \) with \( 0 \leq i < j \leq k \). This implies that if \( \nabla J_{u_i} \neq 0 \) for \( i = 0, \ldots, k \), then the vectors \( \nabla J_{u_i} \) are linearly independent, so the method stops in at most \( n \) steps.

(b) If we write \( \Delta_\ell = u_{\ell+1} - u_\ell = -\rho_\ell d_\ell \), the second remarkable fact about the conjugate gradient method is that the vectors \( \Delta_\ell \) satisfy the following conditions:

\[
\langle A\Delta_\ell, \Delta_i \rangle = 0 \quad 0 \leq i < \ell \leq k.
\]

The vectors \( \Delta_\ell \) and \( \Delta_i \) are said to be \textit{conjugate} with respect to the matrix \( A \) (or \( A\)-conjugate). As a consequence, if \( \Delta_\ell \neq 0 \) for \( \ell = 0, \ldots, k \), then the vectors \( \Delta_\ell \) are linearly independent.

(c) There is a simple formula to compute \( d_{k+1} \) from \( d_k \), and to compute \( \rho_k \).

We now prove the above facts. We begin with (a).

**Proposition 13.11.** Assume that \( \nabla J_{u_i} \neq 0 \) for \( i = 0, \ldots, k \). Then the minimization problem, find \( u_{k+1} \) such that

\[
u_{k+1} \in u_k + G_k \quad \text{and} \quad J(u_{k+1}) = \inf_{v \in u_k + G_k} J(v),
\]

has a unique solution, and the gradients \( \nabla J_{u_i} \) and \( \nabla J_{u_j} \) are orthogonal for all \( i, j \) with \( 0 \leq i < j \leq k \).

**Proof.** The affine space \( u_\ell + G_\ell \) is closed and convex, and since \( J \) is a quadratic elliptic functional it is coercive and strictly convex, so by Theorem 30.7(2) it has a unique minimum in \( u_\ell + G_\ell \). This minimum \( u_{\ell+1} \) is also the minimum of the problem, find \( u_{\ell+1} \) such that

\[
u_{\ell+1} \in u_\ell + G_\ell \quad \text{and} \quad J(u_{\ell+1}) = \inf_{v \in G_\ell} J(u_\ell + v),
\]

and since \( G_\ell \) is a vector space, by Theorem 21.8 we must have

\[
d_{J_{u_\ell}}(w) = 0 \quad \text{for all} \ w \in G_\ell,
\]

that is

\[
\langle \nabla J_{u_\ell}, w \rangle = 0 \quad \text{for all} \ w \in G_\ell.
\]

Since \( G_\ell \) is spanned by \( (\nabla J_{u_0}, \nabla J_{u_1}, \ldots, \nabla J_{u_\ell}) \), we obtain

\[
\langle \nabla J_{u_\ell}, \nabla J_{u_j} \rangle = 0, \quad 0 \leq j < \ell,
\]
and since this holds for $\ell = 0, \ldots, k$, we get

$$\langle \nabla J_{u_i}, \nabla J_{u_j} \rangle = 0, \quad 0 \leq i < j \leq k,$$

which shows the second part of the proposition.

As a corollary of Proposition 30.11, if $\nabla J_{u_i} \neq 0$ for $i = 0, \ldots, k$, then the vectors $\nabla J_{u_i}$ are linearly independent and $G_k$ has dimension $k + 1$. Therefore, the conjugate gradient method terminates in at most $n$ steps. Here is an example of a problem for which the gradient descent with optimal stepsize parameter does not converge in a finite number of steps.

Example 13.1. Let $J: \mathbb{R}^2 \rightarrow \mathbb{R}$ be the function given by

$$J(v_1, v_2) = \frac{1}{2}(\alpha_1 v_1^2 + \alpha_2 v_2^2),$$

where $0 < \alpha_1 < \alpha_2$. The minimum of $J$ is attained at $(0, 0)$. Unless the initial vector $u_0 = (u_0^0, u_0^0)$ has the property that either $u_0^0 = 0$ or $u_0^0 = 0$, we claim that the gradient descent with optimal stepsize parameter does not converge in a finite number of steps. Observe that

$$\nabla J(v_1, v_2) = \begin{pmatrix} \alpha_1 v_1 \\ \alpha_2 v_2 \end{pmatrix}.$$

As a consequence, given $u_k$, the line search for finding $\rho_k$ and $u_{k+1}$ yields $u_{k+1} = (0, 0)$ iff there is some $\rho \in \mathbb{R}$ such that

$$u_1^k = \rho \alpha_1 u_1^k \quad \text{and} \quad u_2^k = \rho \alpha_2 u_2^k.$$

Since $\alpha_1 \neq \alpha_2$, this is only possible if either $u_1^k = 0$ or $u_2^k = 0$. The formulae given just before Proposition 30.10 yield

$$u_1^{k+1} = \frac{\alpha_2^2(\alpha_2 - \alpha_1)u_1^k u_2^k}{\alpha_1^3(u_1^k)^2 + \alpha_2^3(u_2^k)^2}, \quad u_2^{k+1} = \frac{\alpha_1^2(\alpha_1 - \alpha_2)u_2^k u_1^k}{\alpha_1^3(u_1^k)^2 + \alpha_2^3(u_2^k)^2},$$

which implies that if $u_1^k \neq 0$ and $u_2^k \neq 0$, then $u_1^{k+1} \neq 0$ and $u_2^{k+1} \neq 0$, so the method runs forever from any initial vector $u_0 = (u_0^0, u_0^0)$ such that $u_0^0 \neq 0$ and $u_0^0 \neq 0$.

We now prove (b).

Proposition 13.12. Assume that $\nabla J_{u_i} \neq 0$ for $i = 0, \ldots, k$, and let $\Delta_\ell = u_{\ell+1} - u_\ell$, for $\ell = 0, \ldots, k$. Then $\Delta_\ell \neq 0$ for $\ell = 0, \ldots, k$, and

$$\langle A \Delta_\ell, \Delta_i \rangle = 0, \quad 0 \leq i < \ell \leq k.$$

The vectors $\Delta_0, \ldots, \Delta_k$ are linearly independent.
Proof. Since $J$ is a quadratic functional we have

$$\nabla J_{v+w} = A(v+w) - b = Av - b + Aw = \nabla J_v + Aw.$$  

It follows that

$$\nabla J_{u_{\ell+1}} = \nabla J_{u_{\ell+\Delta \ell}} = \nabla J_{u_{\ell}} + A\Delta \ell, \quad 0 \leq \ell \leq k.$$  \hspace{1cm} (*)

By Proposition 30.11, since

$$\langle \nabla J_{u_i}, \nabla J_{u_j} \rangle = 0, \quad 0 \leq i < j \leq k,$$

we get

$$0 = \langle \nabla J_{u_{\ell+1}}, \nabla J_{u_{\ell}} \rangle = \|\nabla J_{u_{\ell}}\|^2 + \langle A\Delta \ell, \nabla J_{u_{\ell}} \rangle, \quad \ell = 0, \ldots, k,$$

and since by hypothesis $\nabla J_{u_i} \neq 0$ for $i = 0, \ldots, k$, we deduce that

$$\Delta \ell \neq 0, \quad \ell = 0, \ldots, k.$$  

If $k \geq 1$, for $i = 0, \ldots, \ell - 1$ and $\ell \leq k$ we also have

$$0 = \langle \nabla J_{u_{\ell+1}}, \nabla J_{u_{\ell}} \rangle = \langle \nabla J_{u_{\ell}}, \nabla J_{u_{\ell+1}} \rangle + \langle A\Delta \ell, \nabla J_{u_{\ell}} \rangle = \langle A\Delta \ell, \nabla J_{u_{\ell}} \rangle.$$  

Since $\Delta_j = u_{j+1} - u_j \in G_j$ and $G_j$ is spanned by $(\nabla J_{u_0}, \nabla J_{u_1}, \ldots, \nabla J_{u_j})$, we obtain

$$\langle A\Delta \ell, \Delta_j \rangle = 0, \quad 0 \leq j < \ell \leq k.$$  

For the last statement of the proposition, let $w_0, w_1, \ldots, w_k$ be any $k+1$ nonzero vectors such that

$$\langle Aw_i, w_j \rangle = 0, \quad 0 \leq i < j \leq k.$$  

We claim that $w_0, w_1, \ldots, w_k$ are linearly independent.

If we have a linear dependence $\sum_{i=0}^k \lambda_i w_i = 0$, then we have

$$0 = \left\langle A \left( \sum_{i=0}^k \lambda_i w_i \right), w_j \right\rangle = \sum_{i=0}^k \lambda_i \langle Aw_i, w_j \rangle = \lambda_j \langle Aw_j, w_j \rangle.$$  

Since $A$ is symmetric positive definite (because $J$ is a quadratic elliptic functional) and $w_j \neq 0$, we must have $\lambda_j = 0$ for $j = 0, \ldots, k$. Therefore the vectors $w_0, w_1, \ldots, w_k$ are linearly independent.  \hfill $\square$

Remarks:

(1) Since $A$ is symmetric positive definite, the bilinear map $(u, v) \mapsto \langle Au, v \rangle$ is an inner product $\langle -, - \rangle_A$ on $\mathbb{R}^n$. Consequently, two vectors $u, v$ are conjugate with respect to the matrix $A$ (or $A$-conjugate), which means that $\langle Au, v \rangle = 0$, iff $u$ and $v$ are orthogonal with respect to the inner product $\langle -, - \rangle_A$.  

(2) By picking the descent direction to be $-\nabla J_{u_k}$, the gradient descent method with optimal stepsize parameter treats the level sets $\{u \mid J(u) = J(u_k)\}$ as if they were spheres. The conjugate gradient method is more subtle, and takes the “geometry” of the level set $\{u \mid J(u) = J(u_k)\}$ into account, through the notion of conjugate directions.

(3) The notion of conjugate direction has its origins in the theory of projective conics and quadrics where $A$ is a $2 \times 2$ or a $3 \times 3$ matrix and where $u$ and $v$ are conjugate iff $u^\top Av = 0$.

(4) The terminology conjugate gradient is somewhat misleading. It is not the gradients who are conjugate directions, but the descent directions.

By definition of the vectors $\Delta_\ell = u_{\ell+1} - u_\ell$, we can write

$$\Delta_\ell = \sum_{i=0}^{\ell} \delta_\ell^i \nabla J_{u_i}, \quad 0 \leq \ell \leq k. \quad (**_2)$$

In matrix form, we can write

$$\begin{pmatrix} \Delta_0 & \Delta_1 & \cdots & \Delta_k \end{pmatrix} = \begin{pmatrix} \nabla J_{u_0} & \nabla J_{u_1} & \cdots & \nabla J_{u_k} \end{pmatrix} \begin{pmatrix} \delta_0^0 & \delta_0^1 & \cdots & \delta_0^{k-1} & \delta_0^k \\ 0 & \delta_1^0 & \cdots & \delta_1^{k-1} & \delta_1^k \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & \delta_k^k \end{pmatrix},$$

which implies that $\delta_\ell^\ell \neq 0$ for $\ell = 0, \ldots, k$.

In view of the above fact, since $\Delta_\ell$ and $d_\ell$ are collinear, it is convenient to write the descent direction $d_\ell$ as

$$d_\ell = \sum_{i=0}^{\ell-1} \lambda_\ell^i \nabla J_{u_i} + \nabla J_{u_\ell}, \quad 0 \leq \ell \leq k. \quad (**_3)$$

Our next goal is to compute $u_{k+1}$, assuming that the coefficients $\lambda_\ell^i$ are known for $i = 0, \ldots, k$, and then to find simple formulae for the $\lambda_\ell^i$.

The problem reduces to finding $\rho_k$ such that

$$J(u_k - \rho_k d_k) = \inf_{\rho \in \mathbb{R}} J(u_k - \rho d_k),$$

and then $u_{k+1} = u_k - \rho_k d_k$. In fact, by (**2), since

$$\Delta_k = \sum_{i=0}^{k} \delta_k^i \nabla J_{u_i} = \delta_k^k \left( \sum_{i=0}^{k-1} \delta_k^i \nabla J_{u_i} + \nabla J_{u_k} \right),$$
we must have
\[ \Delta_k = \delta_k^k d_k \quad \text{and} \quad \rho_k = -\delta_k^k. \] (*4)

Remarkably, the coefficients \( \lambda_i^k \) and the descent directions \( d_k \) can be computed easily using the following formulae.

**Proposition 13.13.** Assume that \( \nabla J_{u_i} \neq 0 \) for \( i = 0, \ldots, k \). If we write
\[ d_\ell = \sum_{i=0}^{\ell-1} \lambda_i^\ell \nabla J_{u_i} + \nabla J_{u_\ell}, \quad 0 \leq \ell \leq k, \]
then we have
\[
\begin{cases}
\lambda_i^k = \frac{\|\nabla J_{u_i}\|^2}{\|\nabla J_{u_i}\|}, & 0 \leq i \leq k - 1, \\
d_0 = \nabla J_{u_0}, \\
d_\ell = \nabla J_{u_\ell} + \frac{\|\nabla J_{u_{\ell+1}}\|^2}{\|\nabla J_{u_{\ell+1}}\|^2} d_{\ell-1}, & 1 \leq \ell \leq k.
\end{cases}
\]

**Proof.** Since by (*4) we have \( \Delta_k = \delta_k^k d_k, \delta_k^k \neq 0 \), (by Proposition 30.12) we have
\[ \langle A \Delta_\ell, \Delta_i \rangle = 0, \quad 0 \leq i < \ell \leq k, \]
by (*1) we have \( \nabla J_{u_{\ell+1}} = \nabla J_{u_\ell} + A \Delta_\ell \), and \( A \) is a symmetric matrix, we have
\[ 0 = \langle Ad_k, \Delta_\ell \rangle = \langle d_k, A \Delta_\ell \rangle = \langle d_k, \nabla J_{u_{\ell+1}} - \nabla J_{u_\ell} \rangle, \]
for \( \ell = 0, \ldots, k - 1 \), and since
\[ d_k = \sum_{i=0}^{k-1} \lambda_i^k \nabla J_{u_i} + \nabla J_{u_k}, \]
we have
\[ \left\langle \sum_{i=0}^{k-1} \lambda_i^k \nabla J_{u_i} + \nabla J_{u_k}, \nabla J_{u_{\ell+1}} - \nabla J_{u_\ell} \right\rangle = 0, \quad 0 \leq \ell \leq k - 1. \]
Since by Proposition 30.11 the gradients \( \nabla J_{u_i} \) are pairwise orthogonal, the above equations yield
\[ -\lambda_{k-1}^k \|\nabla J_{u_{k-1}}\|^2 + \|\nabla J_k\|^2 = 0 \]
\[ -\lambda_\ell^k \|\nabla J_{u_\ell}\|^2 + \lambda_{\ell+1}^k \|\nabla J_{\ell+1}\|^2 = 0, \quad 0 \leq \ell \leq k - 2, \quad k \geq 2, \]
and an easy induction yields
\[ \lambda_i^k = \frac{\|\nabla J_{u_k}\|^2}{\|\nabla J_{u_i}\|^2}, \quad 0 \leq i \leq k - 1. \]
Consequently, using $(\ast_3)$ we have

\[
d_k = \sum_{i=0}^{k-1} \frac{\|\nabla J_{u_k}\|^2}{\|\nabla J_{u_i}\|^2} \nabla J_{u_i} + \nabla J_{u_k}
\]

\[
= \nabla J_{u_k} + \left( \sum_{i=0}^{k-2} \frac{\|\nabla J_{u_{k-1}}\|^2}{\|\nabla J_{u_i}\|^2} \nabla J_{u_i} + \nabla J_{u_{k-1}} \right)
\]

\[
= \nabla J_{u_k} + \frac{\|\nabla J_{u_k}\|^2}{\|\nabla J_{u_{k-1}}\|^2} d_{k-1},
\]

which concludes the proof.

It remains to compute $\rho_k$, which is the solution of the line search

\[
J(u_k - \rho_k d_k) = \inf_{\rho \in \mathbb{R}} J(u_k - \rho d_k).
\]

Since $J$ is a quadratic functional, the function to be minimized is

\[
\rho \mapsto \frac{\rho^2}{2} \langle Ad_k, d_k \rangle - \rho \langle \nabla J_{u_k}, d_k \rangle + J(u_k),
\]

whose minimum is obtained when its derivative is zero, that is,

\[
\rho_k = \frac{\langle \nabla J_{u_k}, d_k \rangle}{\langle Ad_k, d_k \rangle}.
\] (\ast_5)

In summary, the conjugate gradient method finds the minimum $u$ of the elliptic quadratic functional

\[
J(v) = \frac{1}{2} \langle Av, a \rangle - \langle b, v \rangle
\]

by computing the sequence of vectors $u_1, d_1, \ldots, u_{k-1}, d_{k-1}, u_k$, starting from any vector $u_0$, with

\[
d_0 = \nabla J_{u_0}.
\]

If $\nabla J_{u_0} = 0$, then the algorithm terminates with $u = u_0$. Otherwise, for $k \geq 0$, assuming that $\nabla J_{u_i} \neq 0$ for $i = 1, \ldots, k$, compute

\[
\begin{cases}
\rho_k = \frac{\langle \nabla J_{u_k}, d_k \rangle}{\langle Ad_k, d_k \rangle} \\
u_{k+1} = u_k - \rho_k d_k \\
d_{k+1} = \nabla J_{u_{k+1}} + \frac{\|\nabla J_{u_{k+1}}\|^2}{\|\nabla J_{u_k}\|^2} d_k.
\end{cases}
\] (\ast_6)

If $\nabla J_{u_{k+1}} = 0$, then the algorithm terminates with $u = u_{k+1}$. 

\[
\rho_k = \frac{\langle \nabla J_{u_k}, d_k \rangle}{\langle Ad_k, d_k \rangle} \\
u_{k+1} = u_k - \rho_k d_k \\
d_{k+1} = \nabla J_{u_{k+1}} + \frac{\|\nabla J_{u_{k+1}}\|^2}{\|\nabla J_{u_k}\|^2} d_k.
\]
As we showed before, the algorithm terminates in at most \( n \) iterations.

Hestenes and Stiefel realized that the equations (\( \ast_6 \)) can be modified to make the computations more efficient, by having only one evaluation of the matrix \( A \) on a vector, namely \( d_k \). The idea is to compute \( \nabla u_k \) inductively.

Since by (\( \ast_1 \)) and (\( \ast_4 \)) we have
\[
\nabla J_{u_{\ell+1}} = \nabla J_{u_\ell} + A\Delta_\ell = \nabla J_{u_\ell} - \rho_k Ad_k,
\]
the gradient \( \nabla J_{u_{\ell+1}} \) can be computed iteratively:
\[
\begin{align*}
\nabla J_0 &= Au_0 - b \\
\nabla J_{u_\ell+1} &= \nabla J_{u_\ell} - \rho_k Ad_k.
\end{align*}
\]

Since by Proposition 30.13 we have
\[
d_k = \nabla J_{u_k} + \frac{\| \nabla J_{u_k} \|^2}{\| \nabla J_{u_{k-1}} \|^2} d_{k-1}
\]
and since \( d_{k-1} \) is a linear combination of the gradients \( \nabla J_{u_i} \) for \( i = 0, \ldots, k - 1 \), which are all orthogonal to \( \nabla J_{u_k} \), we have
\[
\rho_k = \frac{\langle \nabla J_{u_k}, d_k \rangle}{\langle Ad_k, d_k \rangle} = \frac{\| \nabla J_{u_k} \|^2}{\langle Ad_k, d_k \rangle}.
\]

It is customary to introduce the term \( r_k \) defined as
\[
\nabla J_{u_k} = Au_k - b \quad (\ast_7)
\]
and to call it the residual. Then the conjugate gradient method consists of the following steps. We initialize the method starting from any vector \( u_0 \) and set
\[
d_0 = r_0 = Au_0 - b.
\]

The main iteration step is \( (k \geq 0) \):
\[
\begin{align*}
\rho_k &= \frac{\| r_k \|^2}{\langle Ad_k, d_k \rangle} \\
u_{k+1} &= u_k - \rho_k d_k \\
r_{k+1} &= r_k - \rho_k Ad_k \\
\beta_{k+1} &= \frac{\| r_{k+1} \|^2}{\| r_k \|^2} \\
d_{k+1} &= r_{k+1} + \beta_{k+1} d_k.
\end{align*}
\]

Beware that some authors define the residual \( r_k \) as \( r_k = b - Au_k \) and the descent direction \( d_k \) as \( -d_k \). In this case, the second equation becomes
\[
u_{k+1} = u_k + \rho_k d_k.
\]
Since \( d_0 = r_0 \), the equations
\[
\begin{align*}
r_{k+1} &= r_k - \rho_k A d_k \\
d_{k+1} &= r_{k+1} - \beta_{k+1} d_k
\end{align*}
\]

imply by induction that the subspace \( \mathcal{G}_k \) spanned by \( (r_0, r_1, \ldots, r_k) \) and \( (d_0, d_1, \ldots, d_k) \) is the subspace spanned by \( (r_0, Ar_0, A^2 r_0, \ldots, A^k r_0) \).
Such a subspace is called a Krylov subspace.

If we define the error \( e_k \) as \( e_k = u_k - u \), then \( e_0 = u_0 - u \) and \( Ae_0 = Au_0 - Au = Au_0 - b = d_0 = r_0 \), and then because
\[
u_{k+1} = u_k - \rho_k d_k
\]
we see that \( e_{k+1} = e_k - \rho_k d_k \).
Since \( d_k \) belongs to the subspace spanned by \( (r_0, Ar_0, A^2 r_0, \ldots, A^k r_0) \) and \( r_0 = Ae_0 \), we see that \( d_k \) belongs to the subspace spanned by \( (Ae_0, A^2 e_0, A^3 e_0, \ldots, A^{k+1} e_0) \), and then by induction we see that \( e_{k+1} \) belongs to the subspace spanned by \( (e_0, Ae_0, A^2 e_0, A^3 e_0, \ldots, A^{k+1} e_0) \).
This means that there is a polynomial \( P_k \) of degree \( \leq k \) such that \( P_k(0) = 1 \) and
\[
e_k = P_k(A)e_0.
\]

This is an important fact because it allows an analysis of the convergence of the conjugate gradient method; see Trefethen and Bau [106] (Lecture 38). For this, since \( A \) is symmetric positive definite, we know that \( \lambda \) is a symmetric positive definite matrix it has real positive eigenvalues
\[\lambda_1, \ldots, \lambda_n\]
and there is an orthonormal basis of eigenvectors \( h_1, \ldots, h_n \) so that if we write \( e_0 = \sum_{j=1}^n a_j h_j \), then we have
\[
\|e_0\|_A^2 = \langle Ae_0, e_0 \rangle = \left\langle \sum_{i=1}^n a_i \lambda_i h_i, \sum_{j=1}^n a_j h_j \right\rangle = \sum_{j=1}^n a_j^2 \lambda_j
\]
and

\[\|P(A)e_0\|_A^2 = \langle AP(A)e_0, P(A)e_0 \rangle = \left( \sum_{i=1}^{n} a_i \lambda_i P(\lambda_i) h_i, \sum_{j=1}^{n} a_j P(\lambda_j) h_j \right) = \sum_{j=1}^{n} a_j^2 \lambda_j (P(\lambda_j))^2.\]

These equations imply that

\[\|e_k\|_A \leq \left( \inf_{P \in P_k} \max_{1 \leq i \leq n} |P(\lambda_i)| \right) \|e_0\|_A.\]

It can be shown that the conjugate gradient method requires of the order of

- \(n^3\) additions,
- \(n^3\) multiplications,
- \(2n\) divisions.

In theory, this is worse than the number of elementary operations required by the Cholesky method. Even though the conjugate gradient method does not seem to be the best method for full matrices, it usually outperforms other methods for sparse matrices. The reason is that the matrix \(A\) only appears in the computation of the vector \(Ad_k\). If the matrix \(A\) is banded (for example, tridiagonal), computing \(Ad_k\) is very cheap and there is no need to store the entire matrix \(A\), in which case the conjugate gradient method is fast. Also, although in theory, up to \(n\) iterations may be required, in practice, convergence may occur after a much smaller number of iterations.

Using the inequality

\[\|e_k\|_A \leq \left( \inf_{P \in P_k} \max_{1 \leq i \leq n} |P(\lambda_i)| \right) \|e_0\|_A,\]

by choosing \(P\) to be shifted Chebyshev polynomial, it can be shown that

\[\|e_k\|_A \leq 2 \left( \frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1} \right)^k \|e_0\|_A,\]

where \(\kappa = \text{cond}_2(A)\); see Trefethen and Bau [106] (Lecture 38, Theorem 38.5). Thus the rate of convergence of the conjugate gradient method is governed by the ratio

\[\frac{\sqrt{\text{cond}_2(A)} - 1}{\sqrt{\text{cond}_2(A)} + 1},\]

where \(\text{cond}_2(A) = \lambda_m/\lambda_1\) is the condition number of the matrix \(A\). Since \(A\) is positive definite, \(\lambda_1\) is its smallest eigenvalue and \(\lambda_m\) is its largest eigenvalue.

The above fact leads to the process of preconditioning, a method which consists in replacing the matrix of a linear system \(Ax = b\) by an “equivalent” one for example \(M^{-1}A\) (since
$M$ is invertible, the system $Ax = b$ is equivalent to the system $M^{-1}Ax = M^{-1}b$), where $M$ is chosen so that $M^{-1}A$ is still symmetric positive definite and has a smaller condition number than $A$; see Trefethen and Bau [106] (Lecture 40) and Demmel [33] (Section 6.6.5).

The method of conjugate gradients can be generalized to functionals that are not necessarily quadratic. The stepsize parameter $\rho_k$ is still determined by a line search which consists in finding $\rho_k$ such that

$$J(u_k - \rho_k d_k) = \inf_{\rho \in \mathbb{R}} J(u_k - \rho d_k).$$

This is more difficult than in the quadratic case and in general there is no guarantee that $\rho_k$ is unique, so some criterion to pick $\rho_k$ is needed. Then

$$u_{k+1} = u_k - \rho_k d_k,$$

and the next descent direction can be chosen in two ways:

1. (Polak–Ribière)

$$d_k = \nabla J_{u_k} + \frac{\langle \nabla J_{u_k}, \nabla J_{u_k} - \nabla J_{u_{k-1}} \rangle}{\|\nabla J_{u_{k-1}}\|^2} d_{k-1},$$

2. (Fletcher–Reeves)

$$d_k = \nabla J_{u_k} + \frac{\|\nabla J_{u_k}\|^2}{\|\nabla J_{u_{k-1}}\|^2} d_{k-1}.$$

Consecutive gradients are no longer orthogonal so these methods may run forever. There are various sufficient criteria for convergence. In practice, the Polak–Ribière method converges faster. There no longer any guarantee that these methods converge to a global minimum.

13.4 Gradient Projection Methods for Constrained Optimization

We now consider the problem of finding the minimum of a convex functional $J : V \to \mathbb{R}$ over a nonempty convex subset $U$ of a Hilbert space $V$. By Theorem 21.11(3), the functional $J$ has a minimum at $u \in U$ iff

$$dJ_u(v - u) \geq 0 \quad \text{for all } v \in U,$$

which can be expressed as

$$\langle \nabla J_u, v - u \rangle \geq 0 \quad \text{for all } v \in U.$$
On the other hand, by the projection lemma (Proposition 29.5), the condition for a vector $u \in U$ to be the projection of an element $w \in V$ onto $U$ is

$$\langle u - w, v - u \rangle \geq 0 \quad \text{for all } v \in U.$$  

These conditions are obviously analogous, and we can make this analogy more precise as follows. If $p_U : V \to U$ is the projection map onto $U$, we have the following chain of equivalences:

$$u \in U \quad \text{and} \quad J(u) = \inf_{v \in U} J(v) \iff u \in U \quad \text{and} \quad \langle \nabla J_u, v - u \rangle \geq 0 \quad \text{for every } v \in U,$$

$$u \in U \quad \text{and} \quad \langle u - (u - \rho \nabla J_u), v - u \rangle \geq 0 \quad \text{for every } u, v \in U \text{ and every } \rho > 0,$$

$$u = p_U(u - \rho \nabla J_u) \quad \text{for every } \rho > 0.$$

In other words, for every $\rho > 0$, $u \in V$ is a fixed-point of the function $g : V \to U$ given by

$$g(v) = p_U(v - \rho \nabla J_v).$$

The above suggests finding $u$ by the method of successive approximations for finding the fixed-point of a contracting mapping, namely given any initial $u_0 \in V$, to define the sequence $(u_k)_{k \geq 0}$ such that

$$u_{k+1} = p_U(u_k - \rho_k \nabla J_{u_k}),$$

where the parameter $\rho_k > 0$ is chosen at each step. This method is called the projected-gradient method with variable stepsize parameter. Observe that if $U = V$, then this is just the gradient method with variable stepsize. We have the following result about the convergence of this method.

**Proposition 13.14.** Let $J : V \to \mathbb{R}$ be a continuously differentiable functional defined on a Hilbert space $V$, and let $U$ be nonempty, convex, closed subset of $V$. Suppose there exists two constants $\alpha > 0$ and $M > 0$ such that

$$\langle \nabla J_v - \nabla J_u, v - u \rangle \geq \alpha \|v - u\|^2 \quad \text{for all } u, v \in V,$$

and

$$\|\nabla J_v - \nabla J_u\| \leq M \|v - u\| \quad \text{for all } u, v \in V.$$  

If there exists two real numbers $a, b \in \mathbb{R}$ such that

$$0 < a \leq \rho_k \leq b \leq \frac{2\alpha}{M^2} \quad \text{for all } k \geq 0,$$

then the projected-gradient method with variable stepsize parameter converges. Furthermore, there is some constant $\beta > 0$ (depending on $\alpha, M, a, b$) such that

$$\beta < 1 \quad \text{and} \quad \|u_k - u\| \leq \beta^k \|u_0 - u\|,$$

where $u \in M$ is the unique minimum of $J$. 

Proof. For every $\geq 0$, define the function $g_k : V \to U$ by
\[ g_k(v) = p_U(v - \rho_k \nabla J_v). \]
By Proposition 29.6, the projection map $p_U$ has Lipschitz constant 1, so using the inequalities assumed to hold in the proposition, we have
\[
\|g_k(v_1) - g_k(v_2)\|^2 = \|p_U(v_1 - \rho_k \nabla J_{v_1}) - p_U(v_2 - \rho_k \nabla J_{v_2})\|^2 \\
\leq \|(v_1 - v_2) - \rho_k(\nabla J_{v_1} - \nabla J_{v_2})\|^2 \\
= \|v_1 - v_2\|^2 - 2\rho_k \langle \nabla J_{v_1} - \nabla J_{v_2}, v_1 - v_2 \rangle + \rho_k^2 \|\nabla J_{v_1} - \nabla J_{v_2}\|^2 \\
\leq \left(1 - 2\alpha \rho_k + M^2 \rho_k^2\right) \|v_1 - v_2\|^2.
\]
As in the proof of Proposition 30.10, we know that if $a$ and $b$ satisfy the conditions $0 < a \leq \rho_k \leq b \leq \frac{2\lambda}{M^2}$, then there is some $\beta$ such that
\[
\left(1 - 2\alpha \rho_k + M^2 \rho_k^2\right)^{1/2} \leq \beta < 1 \quad \text{for all } k \geq 0.
\]
Since the minimizing point $u \in U$ is a fixed point of $g_k$ for all $k$, by letting $v_1 = u_k$ and $v_2 = u$, we get
\[
\|u_{k+1} - u\| = \|g_k(u_k) - g_k(u)\| \leq \beta \|u_k - u\|,
\]
which proves the convergence of the sequence $(u_k)_{k \geq 0}$. \hfill \qed

In the case of an elliptic quadratic functional
\[ J(v) = \frac{1}{2} \langle Av, a \rangle - \langle b, v \rangle \]
defined on $\mathbb{R}^n$, the reasoning just after the proof of Proposition 30.10 can be immediately adapted to show that convergence takes place as long as $a, b$ and $\rho_k$ are chosen such that
\[ 0 < a \leq \rho_k \leq b \leq \frac{2}{\lambda_n}. \]

In theory, Proposition 30.14 gives a guarantee of the convergence of the projected-gradient method. Unfortunately, because computing the projection $p_U(v)$ effectively is generally impossible, the range of practical applications of Proposition 30.14 is rather limited. One exception is the case where $U$ is a product $\prod_{i=1}^m [a_i, b_i]$ of closed intervals (where $a_i = -\infty$ or $b_i = +\infty$ is possible). In this case, it is not hard to show that
\[
p_U(v)_i = \begin{cases} 
  a_i & \text{if } w_i < a_i \\
  w_i & \text{if } a_i \leq w_i \leq b_i \\
  b_i & \text{if } b_i < w_i.
\end{cases}
\]
In particular, this is the case if

\[ U = \mathbb{R}_+^n = \{ v \in \mathbb{R}^n \mid v \geq 0 \} \]

and if

\[ J(v) = \frac{1}{2} \langle Av, a \rangle - \langle b, v \rangle \]

is an elliptic quadratic functional on \( \mathbb{R}^n \). Then the vector \( u_{k+1} = (u_{1}^{k+1}, \ldots, u_{n}^{k+1}) \) is given in terms of \( u_k = (u_{1}^{k}, \ldots, u_{n}^{k}) \) by

\[ u_{i}^{k+1} = \max\{u_{i}^{k} - \rho_k(Au_k - b)_i, 0\}, \quad 1 \leq i \leq n. \]

### 13.5 Penalty Methods for Constrained Optimization

In the case where \( V = \mathbb{R}^n \), another method to deal with constrained optimization is to incorporate the domain \( U \) into the objective function \( J \) by adding a penalty function.

**Definition 13.6.** Given a nonempty closed convex subset \( U \) of \( \mathbb{R}^n \), a function \( \psi : \mathbb{R}^n \to \mathbb{R} \) is called a **penalty function** for \( U \) if \( \psi \) is convex and continuous and if the following conditions hold:

\[ \psi(v) \geq 0 \text{ for all } v \in \mathbb{R}^n, \text{ and } \psi(v) = 0 \text{ iff } v \in U. \]

The following proposition shows that the use of penalty functions reduces a constrained optimization problem to a sequence of unconstrained optimization problems.

**Proposition 13.15.** Let \( J : \mathbb{R}^n \to \mathbb{R} \) be a continuous, coercive, strictly convex function, \( U \) be a nonempty, convex, closed subset of \( \mathbb{R}^n \), \( \psi : \mathbb{R}^n \to \mathbb{R} \) be a penalty function for \( U \), and let \( J_\epsilon : \mathbb{R}^n \to \mathbb{R} \) be the penalized objective function given by

\[ J_\epsilon(v) = J(v) + \frac{1}{\epsilon} \psi(v) \quad \text{for all } v \in \mathbb{R}^n. \]

Then, for every \( \epsilon > 0 \), there exists a unique element \( u_\epsilon \in \mathbb{R}^n \) such that

\[ J_\epsilon(u_\epsilon) = \inf_{v \in \mathbb{R}^n} J_\epsilon(v). \]

Furthermore, if \( u \in U \) is the unique minimizer of \( J \) over \( U \), so that \( J(u) = \inf_{v \in U} J(v) \), then

\[ \lim_{\epsilon \to 0} u_\epsilon = u. \]

**Proof.** Observe that since \( J \) is coercive, since \( \psi(v) \geq 0 \) for all \( v \in \mathbb{R}^n \), and \( J_\epsilon = J + (1/\epsilon)\psi \), we have \( J_\epsilon(v) \geq J(v) \) for all \( v \in \mathbb{R}^n \), so \( J_\epsilon \) is also coercive. Since \( J \) is strictly convex and \((1/\epsilon)\psi \) is convex, it is immediately checked that \( J_\epsilon = J + (1/\epsilon)\psi \) is also strictly convex. Then by Proposition 30.1 (and the fact that \( J \) and \( J_\epsilon \) are strictly convex), \( J \) has a unique minimizer \( u \in U \), and \( J_\epsilon \) has a unique minimizer \( u_\epsilon \in \mathbb{R}^n \).
13.5. PENALTY METHODS FOR CONSTRAINED OPTIMIZATION

Since $\psi(u) = 0$ iff $u \in U$, and $\psi(v) \geq 0$ for all $v \in \mathbb{R}^n$, we have $J_\epsilon(u) = J(u)$, and since $u_\epsilon$ is the minimizer of $J_\epsilon$ we have $J_\epsilon(u_\epsilon) \leq J_\epsilon(u)$, so we obtain

$$J(u_\epsilon) \leq J(u_\epsilon) + \frac{1}{\epsilon} \psi(u_\epsilon) = J_\epsilon(u_\epsilon) \leq J_\epsilon(u) = J(u),$$

that is,

$$J_\epsilon(u_\epsilon) \leq J(u). \tag{*1}$$

Since $J$ is coercive, the family $(u_\epsilon)_{\epsilon > 0}$ is bounded. By compactness (since we are in $\mathbb{R}^n$), there exists a subsequence $(u_{\epsilon(i)})_{i \geq 0}$ with $\lim_{\epsilon \to \infty} \epsilon(i) = 0$ and some element $u' \in \mathbb{R}^n$ such that

$$\lim_{i \to \infty} u_{\epsilon(i)} = u'.$$

From the inequality $J(u_\epsilon) \leq J(u)$ proved in (*1) and the continuity of $J$, we deduce that

$$J(u') = \lim_{i \to \infty} J(u_{\epsilon(i)}) \leq J(u). \tag{*2}$$

By definition of $J_\epsilon(u_\epsilon)$ and (*1), we have

$$0 \leq \psi(u_{\epsilon(i)}) \leq \epsilon(i) (J(u) - J(u_{\epsilon(i)}),$$

and since the sequence $(u_{\epsilon(i)})_{i \geq 0}$ converges, the numbers $J(u) - J(u_{\epsilon(i)})$ are bounded independently of $i$. Consequently, since $\lim_{i \to \infty} \epsilon(i) = 0$ and since the function $\psi$ is continuous, we have

$$0 = \lim_{i \to \infty} \psi(u_{\epsilon(i)}) = \psi(u'),$$

which shows that $u' \in U$. Since by (*2) we have $J(u') \leq J(u)$, and since both $u, u' \in U$ and $u$ is the unique minimizer of $J$ over $U$ we must have $u' = u$. Therefore $u'$ is the unique minimizer of $J$ over $U$. But then the whole family $(u_\epsilon)_{\epsilon > 0}$ converges to $u$ since we can use the same argument as above for every subsequence of $(u_\epsilon)_{\epsilon > 0}$. □

Note that a convex function $\psi: \mathbb{R}^n \to \mathbb{R}$ is automatically continuous, so the assumption of continuity is redundant.

As an application of Proposition 30.15, if $U$ is given by

$$U = \{v \in \mathbb{R}^n \mid \varphi_i(v) \leq 0, \ i = 1, \ldots, m\},$$

where the functions $\varphi_i: \mathbb{R}^n \to \mathbb{R}$ are convex, we can take $\psi$ to be the function given by

$$\psi(v) = \sum_{i=1}^{m} \max\{\varphi_i(v), 0\}.$$
In practice, the applicability of the penalty-function method is limited by the difficulty to construct effectively “good” functions $\psi$, for example, differentiable ones. Note that in the above example the function $\psi$ is not differentiable. A better penalty function is

$$\psi(v) = \sum_{i=1}^{m} (\max\{\varphi_i(v), 0\})^2.$$  

Another way to deal with constrained optimization problems is to use duality. This approach is investigated in Chapter 31.

13.6 Summary

The main concepts and results of this chapter are listed below:

•
Chapter 14

Introduction to Nonlinear Optimization

In Chapter 21 we investigated the problem of determining when a function $J: \Omega \to \mathbb{R}$ defined on some open subset $\Omega$ of a normed vector space $E$ has a local extremum in a subset $U$ of $\Omega$ defined by equational constraints, namely

$$U = \{ x \in \Omega \mid \varphi_i(x) = 0, \ 1 \leq i \leq m \},$$

where the functions $\varphi_i: \Omega \to \mathbb{R}$ are continuous (and usually, differentiable). Theorem 21.3 gives a necessary condition in terms of the Lagrange multipliers. In Section 21.3, we assume that $U$ is a convex subset of $\Omega$ and Theorem 21.8 gives us a necessary condition for the function $J: \Omega \to \mathbb{R}$ to have a local minimum at $u$ with respect to $U$ if $dJ_u$ exists, namely

$$dJ_u(v - u) \geq 0 \ \text{for all} \ v \in U.$$

Our first goal is to find a necessary criterion for a function $J: \Omega \to \mathbb{R}$ to have a minimum on a subset $U$, even if this subset is not convex. This can be done by introducing a notion of “tangent cone” at a point $u \in U$.

Our approach is very much inspired by Ciarlet [30] because we find it one of the more direct, and it is general enough to accommodate Hilbert spaces. The field of nonlinear optimization and convex optimization is vast and there are many books on the subject. Among those we recommend (in alphabetic order) Bertsekas [13, 14, 15], Bertsekas, Nedić, and Ozdaglar [16], Boyd and Vandenberghe [22], Luenberger [69], and Luenberger and Ye [70].

14.1 The Cone of Feasible Directions

Let $V$ be a normed vector space and let $U$ be a nonempty subset of $V$. For any point $u \in U$, consider any converging sequence $(u_k)_{k \geq 0}$ of vectors $u_k \in U$ having $u$ as their limit, with
$u_k \neq u$ for all $k \geq 0$, and look at the sequence of “unit chords,”

$$\frac{u_k - u}{\|u_k - u\|}.$$ 

This sequence could oscillate forever, or it could have a limit, some unit vector $\hat{w} \in V$. In the second case, all nonzero vectors $\lambda \hat{w}$ for all $\lambda > 0$, belong to the cone of feasible directions at $u$, which is defined as follows.

**Definition 14.1.** Let $V$ be a normed vector space and let $U$ be a nonempty subset of $V$. For any point $u \in U$, the cone $C(u)$ of feasible directions at $u$ is the union of $\{0\}$ and the set of all nonzero vectors $w \in V$ for which there exists some convergent sequence $(u_k)_{k \geq 0}$ of vectors, such that

1. $u_k \in U$ and $u_k \neq u$ for all $k \geq 0$, and $\lim_{k \to \infty} u_k = u$.
2. $\lim_{k \to \infty} \frac{u_k - u}{\|u_k - u\|} = \frac{w}{\|w\|}$, with $w \neq 0$.

Condition (2) can also be expressed as follows: there is a sequence $(\delta_k)_{k \geq 0}$ of vectors $\delta_k \in V$ such that

$u_k = u + \|u_k - u\| \frac{w}{\|w\|} + \|u_k - u\| \delta_k$, $\lim_{k \to \infty} \delta_k = 0$, $w \neq 0$.

Figure 31.1 illustrates the construction of $w$ in $C(u)$.

Figure 14.1: Let $U$ be the pink region in $\mathbb{R}^2$ with fuchsia point $u \in U$. For any sequence $(u_k)_{k \geq 0}$ of points in $U$ which converges to $u$, form the chords $u_k - u$ and take the limit to construct the red vector $w$.

The set $C(u)$ is a cone with apex 0, a notion defined as follows.

**Definition 14.2.** Given a vector space $V$, a nonempty subset $C \subseteq V$ is a cone with apex 0 (for short, a cone), if for any $v \in V$, if $v \in C$, then $\lambda v \in C$ for all $\lambda > 0$ ($\lambda \in \mathbb{R}$). For any $u \in V$, a cone with apex $u$ is any nonempty subset of the form $u + C = \{u + v \mid v \in C\}$, where $C$ is a cone with apex 0; see Figure 31.2.
14.1. THE CONE OF FEASIBLE DIRECTIONS

Figure 14.2: Let $C$ be the cone determined by the bold orange curve through $(0, 0, 1)$ in the plane $z = 1$. Then $u + C$, where $u = (0.25, 0.5, 0.5)$, is the affine translate of $C$ via the vector $u$.

Observe that a cone with apex 0 (or $u$) is not necessarily convex, and that 0 does not necessarily belong to $C$ (resp. $u$ does not necessarily belong to $u + C$), although in the case of the cone of feasible directions $C(u)$ we have $0 \in C(u)$ (and $u \in u + C(u)$). The condition for being a cone only asserts that if a nonzero vector $v$ belongs to $C$, then the open ray $\{\lambda v \mid \lambda > 0\}$ (resp. the affine open ray $u + \{\lambda v \mid \lambda > 0\}$) also belongs to $C$.

Clearly, the cone $C(u)$ of feasible directions at $u$ is a cone with apex 0, and $u + C(u)$ is a cone with apex $u$. Obviously, it would be desirable to have conditions on $U$ that imply that $C(u)$ is a convex cone. Such conditions will be given later on.

Observe that the cone $C(u)$ of feasible directions at $u$ contains the velocity vectors at $u$ of all curves $\gamma$ in $U$ through $u$. If $\gamma: (-1, 1) \to U$ is such a curve with $\gamma(0) = u$, and if $\gamma'(u) \neq 0$ exists, then there is a sequence $(u_k)_{k \geq 0}$ of vectors in $U$ converging to $u$ as in Definition 31.1, with $u_k = \gamma(t_k)$ for some sequence $(t_k)_{k \geq 0}$ of reals $t_k > 0$ such that $\lim_{k \to \infty} t_k = 0$, so that

$$u_k - u = t_k \gamma'(0) + t_k \epsilon_k, \quad \lim_{k \to \infty} \epsilon_k = 0,$$

and we get

$$\lim_{k \to \infty} \frac{u_k - u}{\|u_k - u\|} = \frac{\gamma'(0)}{\|\gamma'(0)\|}.$$

For an illustration of this paragraph in $\mathbb{R}^2$, see Figure 31.3.
Figure 14.3: Let $U$ be purple region in $\mathbb{R}^2$ and $u$ be the designated point on the boundary of $U$. Figure (i.) illustrates two curves through $u$ and two sequences $(u_k)_{k \geq 0}$ converging to $u$. The limit of the chords $u_k - u$ corresponds to the tangent vectors for the appropriate curve. Figure (ii.) illustrates the half plane $C(u)$ of feasible directions.

Example 14.1. In $V = \mathbb{R}^2$, let $\varphi_1$ and $\varphi_2$ be given by

\[
\varphi_1(u_1, u_2) = -u_1 - u_2 \\
\varphi_2(u_1, u_2) = u_1(u_1^2 + u_2^2) - (u_1^2 - u_2^2),
\]

and let

\[
U = \{(u_1, u_2) \in \mathbb{R}^2 \mid \varphi_1(u_1, u_2) \leq 0, \varphi_2(u_1, u_2) \leq 0\}.
\]

The region $U$ shown in Figure 14.4 is bounded by the curve given by the equation $\varphi_1(u_1, u_2) = 0$, that is, $-u_1 - u_2 = 0$, the line of slope $-1$ through the origin, and the curve given by the equation $u_1(u_1^2 + u_2^2) - (u_1^2 - u_2^2) = 0$, a nodal cubic through the origin. We obtain a parametric definition of this curve by letting $u_2 = tu_1$, and we find that

\[
u_1(t) = \frac{1 - t^2}{1 + t^2}, \quad u_2(t) = \frac{t(1 - t^2)}{1 + t^2}.
\]
The tangent vector at $t$ is given by $(u'_1(t), u'_2(t))$ with
\[
u'_1(t) = \frac{-2t(1 + t^2) - (1 - t^2)2t}{(1 + t^2)^2} = \frac{-4t}{(1 + t^2)^2},
\]
and
\[
u'_2(t) = \frac{(1 - 3t^2)(1 + t^2) - (t - t^3)2t}{(1 + t^2)^2} = \frac{1 - 2t^2 - 3t^4 - 2t^2 + 2t^4}{(1 + t^2)^2} = \frac{1 - 4t^2 - t^4}{(1 + t^2)^2}.
\]
The nodal cubic passes through the origin for $t = \pm 1$, and for $t = -1$ the tangent vector is $(1, -1)$, and for $t = 1$ the tangent vector is $(-1, -1)$. The cone of feasible directions $C(0)$ at the origin is given by
\[C(0) = \{(u_1, u_2) \in \mathbb{R}^2 \mid u_1 + u_2 \geq 0, \; |u_1| \geq |u_2|\}.
\]
This is not a convex cone since it contains the sector delimited by the lines $u_2 = u_1$ and $u_2 = -u_1$, but also the ray supported by the vector $(-1, 1)$.

![Figure 14.4](image14.4.png)

Figure 14.4: Figure (i.) illustrates $U$ as the shaded gray region which lies between the line $y = -x$ and nodal cubic. Figure (ii.) shows the cone of feasible directions, $C(0)$, as the union of turquoise triangular cone and the turquoise the directional ray $(-1, 1)$.

The two crucial properties of the cone of feasible directions are shown in the following proposition.

**Proposition 14.1.** Let $U$ be any nonempty subset of a normed vector space $V$. 
(1) For any \( u \in U \), the cone \( C(u) \) of feasible directions at \( u \) is closed.

(2) Let \( J: \Omega \to \mathbb{R} \) be a function defined on an open subset \( \Omega \) containing \( U \). If \( J \) has a local minimum with respect to the set \( U \) at a point \( u \in U \), and if \( J_u' \) exists at \( u \), then

\[
J_u'(v - u) \geq 0 \quad \text{for all } v \in u + C(u).
\]

Proof. (1) Let \( (w_n)_{n \geq 0} \) be a sequence of points \( w_n \in C(u) \) converging to a limit \( w \in V \). We may assume that \( w \neq 0 \), since \( 0 \in C(u) \) by definition, and thus we may also assume that \( w_n \neq 0 \) for all \( n \geq 0 \). By definition, for every \( n \geq 0 \), there is a sequence \( (u^k_n)_{k \geq 0} \) of points in \( V \) and some \( w_n \neq 0 \) such that

\[
(1) \quad u^k_n \in U \text{ and } u^k_n \neq u \text{ for all } k \geq 0, \text{ and } \lim_{k \to \infty} u^k_n = u.
\]

\[
(2) \quad \text{There is a sequence } (\delta^n_k)_{k \geq 0} \text{ of vectors } \delta^n_k \in V \text{ such that}
\]

\[
\begin{aligned}
&u^n_k = u + \|u^n_k - u\| \frac{w_n}{\|w_n\|} + \|u^n_k - u\| \delta^n_k, \\
&\lim_{k \to \infty} \delta^n_k = 0, \quad w_n \neq 0.
\end{aligned}
\]

Let \( (\epsilon_n)_{n \geq 0} \) be a sequence of real numbers \( \epsilon_n > 0 \) such that \( \lim_{n \to \infty} \epsilon_n = 0 \) (for example, \( \epsilon_n = 1/(n + 1) \)). Due to the convergence of the sequences \( (u^n_k) \) and \( (\delta^n_k) \) for every fixed \( n \), there exist an integer \( k(n) \) such that

\[
\|u^n_{k(n)} - u\| \leq \epsilon_n, \quad \|\delta^n_{k(n)}\| \leq \epsilon_n.
\]

Consider the sequence \( (u^n_{k(n)})_{n \geq 0} \). We have

\[
u^n_{k(n)} \in U, \quad u^n_{k(n)} \neq 0, \quad \text{for all } n \geq 0, \quad \lim_{n \to \infty} u^n_{k(n)} = u,
\]

and we can write

\[
u^n_{k(n)} = u + \|u^n_{k(n)} - u\| \frac{w}{\|w\|} + \|u^n_{k(n)} - u\| \left( \delta^n_{k(n)} + \left( \frac{w_n}{\|w_n\|} - \frac{w}{\|w\|} \right) \right).
\]

Since \( \lim_{k \to \infty} (w_n/\|w_n\|) = w/\|w\| \), we conclude that \( w \in C(u) \). See Figure 31.5.

(2) Let \( w = v - u \) be any nonzero vector in the cone \( C(u) \), and let \( (u_k)_{k \geq 0} \) be a sequence of points in \( U - \{u\} \) such that

\[
(1) \quad \lim_{k \to \infty} u_k = u.
\]

\[
(2) \quad \text{There is a sequence } (\delta_k)_{k \geq 0} \text{ of vectors } \delta_k \in V \text{ such that}
\]

\[
u_k - u = \|u_k - u\| \frac{w}{\|w\|} + \|u_k - u\| \delta_k, \quad \lim_{k \to \infty} \delta_k = 0, \quad w \neq 0,
\]

\[
(3) \quad J(u) \leq J(u_k) \text{ for all } k \geq 0.
\]

Figure 14.5: Let $U$ be the mint green region in $\mathbb{R}^2$ with $u = (0, 0)$. Let $(w_n)_{n \geq 0}$ be a sequence of points along the upper dashed curve which converge to $w$. By following the dashed orange longitudinal curves, and selecting an appropriate point, we construct the dark green curve in $U$, which passes through $u$, and at $u$ has tangent vector proportional to $w$.

Since $J$ is differentiable at $u$, we have

$$0 \leq J(u_k) - J(u) = J'_u(u_k - u) + \|u_k - u\| \epsilon_k,$$

for some sequence $(\epsilon_k)_{k \geq 0}$ such that $\lim_{k \to \infty} \epsilon_k = 0$. Since $J'_u$ is linear and continuous, and

$$u_k - u = \|u_k - u\| \frac{w}{\|w\|} + \|u_k - u\| \delta_k, \quad \lim_{k \to \infty} \delta_k = 0, \; w \neq 0,$$

(*) implies that

$$0 \leq \left( \frac{\|u_k - u\|}{\|w\|} (J'_u(w) + \eta_k) \right),$$

with

$$\eta_k = \|w\| (J'_u(\delta_k) + \epsilon_k),$$

and since $J'_u$ is continuous, we have $\lim_{k \to \infty} \eta_k = 0$. But then, $J'_u(w) \geq 0$, since if $J'_u(w) < 0$, then for $k$ large enough the expression $J'_u(w) + \eta_k$ would be negative, and since $u_k \neq u$, the expression $(\|u_k - u\| / \|w\|) (J'_u(w) + \eta_k)$ would also be negative, a contradiction.

From now on, we assume that $U$ is defined by a set of inequalities, that is

$$U = \{x \in \Omega \mid \varphi_i(x) \leq 0, \; 1 \leq i \leq m\},$$

where the functions $\varphi_i : \Omega \to \mathbb{R}$ are continuous (and usually, differentiable). As we explained earlier, an equality constraint $\varphi_i(x) = 0$ is treated as the conjunction of the two inequalities.
ϕ_i(x) ≤ 0 and −ϕ_i(x) ≤ 0. Later on, we will see that when the functions ϕ_i are convex, since −ϕ_i is not necessarily convex, it is desirable to treat equality constraints separately, but for the time being we won’t.

Our next goal is find sufficient conditions for the cone C(u) to be convex, for any u ∈ U. For this, we assume that the functions ϕ_i are differentiable at u. It turns out that the constraints ϕ_i that matter are those for which ϕ_i(u) = 0, namely the constraints that are tight, or as we say, active.

Definition 14.3. Given m functions ϕ_i: Ω → R defined on some open subset Ω of some vector space V, let U be the set defined by

\[ U = \{ x ∈ \Omega \mid ϕ_i(x) ≤ 0, \ 1 ≤ i ≤ m \}. \]

For any u ∈ U, a constraint ϕ_i is said to be active at u if ϕ_i(u) = 0, else inactive at u if ϕ_i(u) < 0.

If a constraint ϕ_i is active at u, this corresponds to u being on a piece of the boundary of U determined by some of the equations ϕ_i(u) = 0; see Figure 31.6.

Definition 14.4. For any u ∈ U, with

\[ U = \{ x ∈ \Omega \mid ϕ_i(x) ≤ 0, \ 1 ≤ i ≤ m \}, \]

we define I(u) as the set of indices

\[ I(u) = \{ i ∈ \{1, \ldots, m\} \mid ϕ_i(u) = 0 \} \]

where the constraints are active. Since each (ϕ_i)'u is a linear form, the subset

\[ C^*(u) = \{ v ∈ V \mid (ϕ_i)'_u(v) ≤ 0, \ i ∈ I(u) \} \]

is the intersection of half spaces passing through the origin, so it is a convex set and obviously it is a cone. If I(u) = ∅, then C^*(u) = V.

The special kinds of H-polyhedra of the form C^*(u) cut out by hyperplanes through the origin are called H-cones. It can be shown that every H-cone is a polyhedral cone (also called a V-cone), and conversely. The proof is nontrivial; see Gallier [45] and Ziegler [114].

We will prove shortly that we always have the inclusion

\[ C(u) ⊆ C^*(u). \]

However, the inclusion can be strict, as in Example 31.1. Indeed for u = (0, 0) we have I(0, 0) = {1, 2} and since

\[ (ϕ'_1)_{(u_1, u_2)} = (-1 \ -1), \quad (ϕ'_2)_{(u_1, u_2)} = (3u_1^2 + u_2^2 - 2u_1 \ 2u_1u_2 + 2u_2), \]

we have (ϕ'_2)_{(0, 0)} = (0 \ 0), and thus C^*(0) = \{(u_1, u_2) ∈ \mathbb{R}^2 \mid u_1 + u_2 ≥ 0\} as illustrated in Figure 31.7.

The conditions stated in the following definition are sufficient conditions that imply that C(u) = C^*(u), as we will prove next.
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Figure 14.6: Let $U$ be the light purple planar region which lies between the curves $y = x^2$ and $y^2 = x$. Figure (i.) illustrates the boundary point $(1, 1)$ given by the equalities $y - x^2 = 0$ and $y^2 - x = 0$. The affine translate of cone of feasible directions, $C(1, 1)$, is illustrated by the pink triangle whose sides are the tangent lines to the boundary curves. Figure (ii.) illustrates the boundary point $(1/4, 1/2)$ given by the equality $y^2 - x = 0$. The affine translate of $C(1/4, 1/2)$ is the lilac half space bounded by the tangent line to $y^2 = x$ through $(1/4, 1/2)$.

Definition 14.5. For any $u \in U$, with

$$U = \{ x \in \Omega \mid \varphi_i(x) \leq 0, \ 1 \leq i \leq m \},$$

if the functions $\varphi_i$ are differentiable at $u$ (in fact, we only this for $i \in I(u)$), we say that the constraints are qualified at $u$ if the following conditions hold:

(a) Either the constraints $\varphi_i$ are affine for all $i \in I(u)$, or

(b) There is some nonzero vector $w \in V$ such that the following conditions hold for all $i \in I(u)$:

(i) $(\varphi'_i)_u(w) \leq 0$. 


Figure 14.7: For $u = (0, 0)$, $C^*(u)$ is the sea green half space given by $u_1 + u_2 \geq 0$. This half space strictly contains $C(u)$, namely union the turquoise triangular cone and directional ray $(-1, 1)$.

(ii) If $\varphi_i$ is not affine, then $(\varphi'_i)^u(w) < 0$.

Condition (b)(ii) implies that $u$ is not a critical point of $\varphi_i$ for every $i \in I(u)$, so there is no singularity at $u$ in the zero locus of $\varphi_i$. Intuitively, if the constraints are qualified at $u$ then the boundary of $U$ near $u$ behaves “nicely.”

The boundary points illustrated in Figure 31.6 are qualified. Observe that $U = \{x \in \mathbb{R}^2 \mid \varphi_1(x, y) = y^2 - x \leq 0, \varphi_2(x, y) = x^2 - y \leq 0\}$. For $u = (1,1)$, $I(u) = \{1, 2\}$, $(\varphi'_1)_{(1,1)} = (-1 2), (\varphi'_2)_{(1,1)} = (2 -1)$, and $w = (-1,1)$ ensures that $(\varphi'_1)_{(1,1)}$ and $(\varphi'_1)_{(1,1)}$ satisfy Condition (b) of Definition 31.5. For $u = (1/4, 1/2)$, $I(u) = \{1\}$, $(\varphi'_1)_{(1,1)} = (-1 1)$, and $w = (-1,0)$ will satisfy Condition (b).

In Example 31.1, the constraint $\varphi_2(u_1, u_2) = 0$ is not qualified at the origin because $(\varphi'_2)_{(0,0)} = (0,0)$; in fact, the origin is a self-intersection. In the example below, the origin is also a singular point, but for a different reason.

**Example 14.2.** Consider the region $U \subseteq \mathbb{R}^2$ determined by the two curves given by

$$\begin{align*}
\varphi_1(u_1, u_2) &= u_2 - \max(0, u_1^2) \\
\varphi_2(u_1, u_2) &= u_1^4 - u_2.
\end{align*}$$

We have $I(0,0) = \{1, 2\}$, and since $(\varphi'_1)_{(0,0)}(w_1, w_2) = (0 1)(w_1 \ w_2) = w_2$ and $(\varphi'_2)_{(0,0)}(w_1, w_2) = (0 -1)(w_1 \ w_2) = -w_2$, we have $C^*(0) = \{(u_1, u_2) \in \mathbb{R}^2 \mid u_2 = 0\}$, but the constraints are not qualified at $(0,0)$ since it is impossible to have simultaneously $(\varphi'_1)_{(0,0)}(w_1, w_2) < 0$ and $(\varphi'_2)_{(0,0)}(w_1, w_2) < 0$, so in fact $C(0) = \{(u_1, u_2) \in \mathbb{R}^2 \mid u_1 \geq 0, u_2 = 0\}$ is strictly contained in $C^*(0)$; see Figure 31.8.
Figure 14.8: Figures (i.) and (ii.) illustrate the purple moon shaped region associated with Example 31.2. Figure (i.) also illustrates $C(0)$, the cone of feasible directions, while Figure (ii.) illustrates the strict containment of $C(0)$ in $C^*(0)$.

**Proposition 14.2.** Let $u$ be any point of the set

$$U = \{ x \in \Omega \mid \phi_i(x) \leq 0, \ 1 \leq i \leq m \},$$

where $\Omega$ is an open subset of the normed vector space $V$, and assume that the functions $\phi_i$ are differentiable at $u$ (in fact, we only this for $i \in I(u)$). Then the following facts hold:

(1) The cone $C(u)$ of feasible directions at $u$ is contained in the convex cone $C^*(u)$; that is,

$$C(u) \subseteq C^*(u) = \{ v \in V \mid (\phi'_i)_u(v) \leq 0, \ i \in I(u) \}.$$

(2) If the constraints are qualified at $u$ (and the functions $\phi_i$ are continuous at $u$ for all $i \notin I(u)$ if we only assume $\phi_i$ differentiable at $u$ for all $i \in I(u)$), then

$$C(u) = C^*(u).$$
Proof. (1) For every \( i \in I(u) \), since \( \varphi_i(v) \leq 0 \) for all \( v \in U \) and \( \varphi_i(u) = 0 \), the function \(-\varphi_i\) has a local minimum at \( u \) with respect to \( U \), so by Proposition 31.1, we have

\[
(-\varphi'_i)_u(v) \geq 0 \quad \text{for all } v \in C(u),
\]

which is equivalent to \((\varphi'_i)_u(v) \leq 0\) for all \( v \in C(u) \) and for all \( i \in I(u) \), that is, \( u \in C^*(u) \).

(2)(a) First, let us assume that \( \varphi_i \) is affine for every \( i \in I(u) \). Recall that \( \varphi_i \) must be given by \( \varphi_i(v) = h_i(v) + c_i \) for all \( v \in V \), where \( h_i \) is a linear form and \( c_i \in \mathbb{R} \). Since the derivative of a linear map at any point is itself,

\[
(\varphi'_i)_u(v) = h_i(v) \quad \text{for all } v \in V.
\]

Pick any nonzero \( w \in C^*(u) \), which means that \((\varphi'_i)_u(w) \leq 0\) for all \( i \in I(u) \). For any sequence \((\epsilon_k)_{k \geq 0}\) of reals \( \epsilon_k > 0 \) such that \( \lim_{k \to \infty} \epsilon_k = 0 \), let \((u_k)_{k \geq 0}\) be the sequence of vectors in \( V \) given by

\[
u_k = u + \epsilon_kw.
\]

We have \( u_k - u = \epsilon_kw \neq 0 \) for all \( k \geq 0 \) and \( \lim_{k \to \infty} u_k = u \). Furthermore, since the functions \( \varphi_i \) are continuous for all \( i \notin I \), we have

\[
0 > \varphi_i(u) = \lim_{k \to \infty} \varphi_i(u_k),
\]

and since \( \varphi_i \) is affine and \( \varphi_i(u) = 0 \) for all \( i \in I \), we have \( \varphi_i(u) = h_i(u) + c_i = 0 \), so

\[
\varphi_i(u_k) = h_i(u_k) + c_i = h_i(u_k) - h_i(u) = h_i(u_k - u) = (\varphi'_i)_u(u_k - u) = \epsilon_k(\varphi'_i)_u(w) \leq 0,
\]

which implies that \( u_k \in U \) for all \( k \) large enough. Since

\[
\frac{u_k - u}{\|u_k - u\|} = \frac{w}{\|w\|} \quad \text{for all } k \geq 0,
\]

we conclude that \( w \in C(u) \). See Figure 31.9.

(2)(b) Let us now consider the case where some function \( \varphi_i \) is not affine for some \( i \in I(u) \). Let \( w \neq 0 \) be some vector in \( V \) such that Condition (b) of Definition 31.5 holds, namely: for all \( i \in I(u) \), we have

(i) \((\varphi'_i)_u(w) \leq 0\).

(ii) If \( \varphi_i \) is not affine, then \((\varphi'_i)_u(w) < 0\).

Pick any nonzero vector \( v \in C^*(u) \), which means that \((\varphi'_i)_u(v) \leq 0\) for all \( i \in I(u) \), and let \( \delta > 0 \) be any positive real number such that \( v + \delta w \neq 0 \). For any sequence \((\epsilon_k)_{k \geq 0}\) of reals \( \epsilon_k > 0 \) such that \( \lim_{k \to \infty} \epsilon_k = 0 \), let \((u_k)_{k \geq 0}\) be the sequence of vectors in \( V \) given by

\[
u_k = u + \epsilon_k(v + \delta w).
\]
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Figure 14.9: Let $U$ be the peach triangle bounded by the lines $y = 0$, $x = 0$, and $y = -x + 1$. Let $u$ satisfy the affine constraint $\varphi(x, y) = y + x - 1$. Since $\varphi'(x,y) = (1\ 1)$, set $w = (-1,-1)$ and approach $u$ along the line $u + tw$.

We have $u_k - u = \epsilon_k(v + \delta w) \neq 0$ for all $k \geq 0$ and $\lim_{k \to \infty} u_k = u$. Furthermore, since the functions $\varphi_i$ are continuous for all $i \notin I(u)$, we have

$$0 > \varphi_i(u) = \lim_{k \to \infty} \varphi_i(u_k) \quad \text{for all } i \notin I(u), \quad (*)_1$$

and as in the previous case, for all $i \in I(u)$ such that $\varphi_i$ is affine, since $(\varphi'_i)_u(v) \leq 0$, $(\varphi'_i)_u(w) \leq 0$, and $\epsilon_k, \delta > 0$, we have

$$\varphi_i(u_k) = \epsilon_k((\varphi'_i)_u(v) + \delta(\varphi'_i)_u(w)) \leq 0 \quad \text{for all } i \in I(u) \text{ and } \varphi_i \text{ affine}, \quad (*)_2$$

and since $\varphi_i$ is differentiable and $\varphi_i(u) = 0$ for all $i \in I(u)$, if $\varphi_i$ is not affine we have

$$\varphi_i(u_k) = \epsilon_k((\varphi'_i)_u(v) + \delta(\varphi'_i)_u(w)) + \epsilon_k \|u_k - u\| \eta_k(u_k - u)$$

with $\lim_{\|u_k - u\| \to 0} \eta_k(u_k - u) = 0$, so if we write $\alpha_k = \|u_k - u\| \eta_k(u_k - u)$, we have

$$\varphi_i(u_k) = \epsilon_k((\varphi'_i)_u(v) + \delta(\varphi'_i)_u(w) + \alpha_k)$$

with $\lim_{k \to \infty} \alpha_k = 0$, and since $(\varphi'_i)_u(v) \leq 0$, we obtain

$$\varphi_i(u_k) \leq \epsilon_k(\delta(\varphi'_i)_u(w) + \alpha_k) \quad \text{for all } i \in I(u) \text{ and } \varphi_i \text{ not affine}. \quad (*)_3$$

The Equations $(*)_1$, $(*)_2$, $(*)_3$ show that $u_k \in U$ for $k$ sufficiently large, where in $(*)_3$, since $(\varphi'_i)_u(w) < 0$ and $\delta > 0$, even if $\alpha_k > 0$, when $\lim_{k \to \infty} \alpha_k = 0$, we will have $\delta(\varphi'_i)_u(w) + \alpha_k < 0$ for $k$ large enough, and thus $\epsilon_k(\delta(\varphi'_i)_u(w) + \alpha_k) < 0$ for $k$ large enough.

Since

$$\frac{u_k - u}{\|u_k - u\|} = \frac{v + \delta w}{\|v + \delta w\|}$$
for all \( k \geq 0 \), we conclude that \( v + \delta w \in C(u) \) for \( \delta > 0 \) small enough. But now the sequence \( (v_n)_{n \geq 0} \) given by
\[
v_n = v + \epsilon_n w
\]
converges to \( v \), and for \( n \) large enough \( v_n \in C(u) \). Since by Proposition 31.1, the cone \( C(u) \) is closed, we conclude that \( v \in C(u) \). See Figure 31.10.

Figure 14.10: Let \( U \) be the pink lounge in \( \mathbb{R}^2 \). Let \( u \) satisfy the non-affine constraint \( \varphi_1(u) \). Choose vectors \( v \) and \( w \) in the half space \( (\varphi_1')_u \leq 0 \). Figure (i.) approaches \( u \) along the line \( u + t(\delta w + v) \) and shows that \( v + \delta w \in C(u) \) for fixed \( \delta \). Figure (ii.) varies \( \delta \) in order that the purple vectors approach \( v \) as \( \delta \to \infty \).

In all cases, we proved that \( C^*(u) \subseteq C(u) \), as claimed.

In the case of \( m \) affine constraints \( a_i x \leq b_i \), for some linear forms \( a_i \) and some \( b_i \in \mathbb{R} \), for any point \( u \in \mathbb{R}^n \) such that \( a_i u = b_i \) for all \( i \in I(u) \), the cone \( C(u) \) consists of all \( v \in \mathbb{R}^n \) such that \( a_i v \leq 0 \), so \( u + C(u) \) consists of all points \( u + v \) such that
\[
a_i(u + v) \leq b_i \quad \text{for all } i \in I(u),
\]
which is the cone cut out by the hyperplanes determining some face of the polyhedron defined
by the \( m \) constraints \( a_i x \leq b_i \).

We are now ready to prove one of the most important results of nonlinear optimization.

### 14.2 The Karush–Kuhn–Tucker Conditions

If the domain \( U \) is defined by inequality constraints satisfying mild differentiability conditions
and if the constraints at \( u \) are qualified, then there is a necessary condition for the function \( J \)
to have a local minimum at \( u \in U \) involving generalized Lagrange multipliers. The proof uses
a version of Farkas Lemma. In fact, the necessary condition stated next holds for infinite-dimensional vector spaces because there a version of Farkas Lemma holding for real Hilbert
spaces, but we will content ourselves with the version holding for finite dimensional normed vector spaces. For the more general version, see Theorem 29.11 (or Ciarlet [30], Chapter 9).

We will be using the following version of Farkas Lemma.

**Proposition 14.3. (Farkas Lemma, Version I)** Let \( A \) be an \( m \times n \) matrix and let \( b \in \mathbb{R}^m \)
be any vector. The linear system \( Ax = b \) has no solution \( x \geq 0 \) iff there is some nonzero
linear form \( y \in (\mathbb{R}^m)^* \) such that \( yA \geq 0^\top_n \) and \( yb < 0 \).

We will use the version of Farkas Lemma obtained by taking a contrapositive, namely:
if \( yA \geq 0^\top_n \) implies \( yb \geq 0 \) for all linear forms \( y \in (\mathbb{R}^m)^* \), then linear system \( Ax = b \) some solution \( x \geq 0 \).

Actually, it is more convenient to use a version of Farkas Lemma applying to a Euclidean
vector space (with an inner product denoted \( \langle -, - \rangle \)). This version also applies to an infinite
dimensional real Hilbert space; see Theorem 29.11. Recall that in a Euclidean space \( V \) the inner product induces an isomorphism between \( V \) and its dual \( V^* \). In our case, we need
the isomorphism \( \# \) from \( V^* \) to \( V \) defined such that for every linear form \( \omega \in V^* \), the vector \( \omega^\# \in V \) is uniquely defined by the equation

\[
\omega(v) = \langle v, \omega^\# \rangle \quad \text{for all } v \in V.
\]

In \( \mathbb{R}^n \), the isomorphism between \( \mathbb{R}^n \) and \( (\mathbb{R}^n)^* \) amounts to transposition: if \( y \in (\mathbb{R}^n)^* \) is
a linear form and \( v \in \mathbb{R}^n \) is a vector, then

\[
yv = v^\top y^\top.
\]

The version of the Farkas–Minskowski lemma in term of an inner product is as follows.

**Proposition 14.4. (Farkas–Minkowski)** Let \( V \) be a Euclidean space of finite dimension with
inner product \( \langle -, - \rangle \) (more generally, a Hilbert space). For any finite family \( (a_1, \ldots, a_m) \) of
\( m \) vectors \( a_i \in V \) and any vector \( b \in V \), for any \( v \in V \),

\[
\text{if } \langle a_i, v \rangle \geq 0 \text{ for } i = 1, \ldots, m \text{ implies that } \langle b, v \rangle \geq 0,
\]
then there exist $\lambda_1, \ldots, \lambda_m \in \mathbb{R}$ such that

$$\lambda_i \geq 0 \text{ for } i = 1, \ldots, m,$$

and

$$b = \sum_{i=1}^{m} \lambda_i a_i,$$

that is, $b$ belong to the polyhedral cone $\text{cone}(a_1, \ldots, a_m)$.

Proposition 31.4 is the special case of Theorem 29.11 which holds for real Hilbert spaces.

We can now prove the following theorem.

**Theorem 14.5.** Let $\varphi_i : \Omega \to \mathbb{R}$ be $m$ constraints defined on some open subset $\Omega$ of a finite-dimensional Euclidean vector space $V$ (more generally, a real Hilbert space $V$), let $J : \Omega \to \mathbb{R}$ be some function, and let $U$ be given by

$$U = \{x \in \Omega \mid \varphi_i(x) \leq 0, \ 1 \leq i \leq m\}.$$

For any $u \in U$, let

$$I(u) = \{i \in \{1, \ldots, m\} \mid \varphi_i(u) = 0\},$$

and assume that the functions $\varphi_i$ are differentiable at $u$ for all $i \in I(u)$ and continuous at $u$ for all $i \notin I(u)$. If $J$ is differentiable at $u$, has a local minimum at $u$ with respect to $U$, and if the constraints are qualified at $u$, then there exist some scalars $\lambda_i(u) \in \mathbb{R}$ for all $i \in I(u)$, such that

$$J_u' + \sum_{i \in I(u)} \lambda_i(u)(\varphi_i')_u = 0, \quad \text{and} \quad \lambda_i(u) \geq 0 \text{ for all } i \in I(u).$$

The above conditions are called the Karush–Kuhn–Tucker optimality conditions. Equivalently, in terms of gradients, the above conditions are expressed as

$$\nabla J_u + \sum_{i \in I(u)} \lambda_i(u)\nabla(\varphi_i)_u = 0, \quad \text{and} \quad \lambda_i(u) \geq 0 \text{ for all } i \in I(u).$$

**Proof.** By Proposition 31.1, we have

$$J_u'(w) \geq 0 \quad \text{for all } w \in C(u), \quad (\ast_1)$$

and by Proposition 31.2, we have $C(u) = C^*(u)$, where

$$C^*(u) = \{v \in V \mid (\varphi_i)_u(v) \leq 0, \ i \in I(u)\}, \quad (\ast_2)$$

so $(\ast_1)$ can be expressed as: for all $w \in V$,

if $w \in C^*(u)$ then $J_u'(w) \geq 0,$

or

if $-(\varphi_i)_u(w) \geq 0$ for all $i \in I(u)$ then $J_u'(w) \geq 0.$ \quad (\ast_3)
Under the isomorphism $\#$, the vector $(J'_u)^{\#}$ is the gradient $\nabla J_u$, so that
\[ J'_u(w) = \langle w, \nabla J_u \rangle, \] (*4)
and the vector $((\varphi'_i)_u)^{\#}$ is the gradient $\nabla (\varphi_i)_u$, so that
\[ (\varphi'_i)_u(w) = \langle w, \nabla (\varphi_i)_u \rangle. \] (*5)

Using the Equations (*4) and (*5), the Equation (*)3 can be written as: for all $w \in V$,
if $\langle w, -\nabla (\varphi_i)_u \rangle \geq 0$ for all $i \in I(u)$ then $\langle w, \nabla J_u \rangle \geq 0$.

By the Farkas–Minkowski proposition (Proposition 31.4), there exist some scalars $\lambda_i(u)$ for all $i \in I(u)$, such that $\lambda_i(u) \geq 0$ and
\[ \nabla J_u = \sum_{i \in I(u)} \lambda_i(u)(-\nabla (\varphi_i)_u), \]
that is
\[ \nabla J_u + \sum_{i \in I(u)} \lambda_i(u)\nabla (\varphi_i)_u = 0, \]
and using the inverse of the isomorphism $\#$ (which is linear), we get
\[ J'_u + \sum_{i \in I(u)} \lambda_i(u)(\varphi'_i)_u = 0, \]
as claimed.

Since the constraints are inequalities of the form $\varphi_i(x) \leq 0$, there is a way of expressing the Karush–Kuhn–Tucker optimality conditions, often abbreviated as KKT conditions, in a way that does not refer explicitly to the index set $I(u)$:
\[ J'_u + \sum_{i=1}^{m} \lambda_i(u)(\varphi'_i)_u = 0, \] (KKT1)
and
\[ \sum_{i=1}^{m} \lambda_i(u)\varphi_i(u) = 0, \quad \lambda_i(u) \geq 0, \quad i = 1, \ldots, m. \] (KKT2)

Indeed, if we have the strict inequality $\varphi_i(u) < 0$ (the constraint $\varphi_i$ is inactive at $u$), since all the terms $\lambda_i(u)\varphi_i(u)$ are nonpositive, we must have $\lambda_i(u) = 0$; that is, we only need to consider the $\lambda_i(u)$ for all $i \in I(u)$. Yet another way to express the conditions in (KKT2) is
\[ \lambda_i(u)\varphi_i(u) = 0, \quad \lambda_i(u) \geq 0, \quad i = 1, \ldots, m. \] (KKT2')
In other words, for any \(i \in \{1, \ldots, m\}\), if \(\varphi_i(u) < 0\), then \(\lambda_i(u) = 0\); that is, if the constraint \(\varphi_i\) is inactive at \(u\), then \(\lambda_i(u) = 0\). By contrapositive, if \(\lambda_i(u) \neq 0\), then \(\varphi_i(u) = 0\); that is, if \(\lambda_i(u) \neq 0\), then the constraint \(\varphi_i\) is active at \(u\). The conditions in (KKT') are referred to as complementary slackness conditions.

The scalars \(\lambda_i(u)\) are often called generalized Lagrange multipliers. If \(V = \mathbb{R}^n\), the necessary conditions of Theorem 31.5 are expressed as the following system of equations and inequalities in the unknowns \((u_1, \ldots, u_n) \in \mathbb{R}^n\) and \((\lambda_1, \ldots, \lambda_m) \in \mathbb{R}_+^m\):

\[
\frac{\partial J}{\partial x_1}(u) + \lambda_1 \frac{\partial \varphi_1}{\partial x_1}(u) + \cdots + \lambda_m \frac{\partial \varphi_m}{\partial x_1}(u) = 0 \\
\vdots \\
\frac{\partial J}{\partial x_n}(u) + \lambda_1 \frac{\partial \varphi_n}{\partial x_1}(u) + \cdots + \lambda_m \frac{\partial \varphi_m}{\partial x_n}(u) = 0 \\
\lambda_1 \varphi_1(u) + \cdots + \lambda_m \varphi_m(u) = 0 \\
\varphi_1(u) \leq 0 \\
\vdots \\
\varphi_m(u) \leq 0 \\
\lambda_1, \ldots, \lambda_m \geq 0.
\]

**Example 14.3.** Let \(J\), \(\varphi_1\) and \(\varphi_2\) be the functions defined on \(\mathbb{R}\) by

\[
J(x) = x \\
\varphi_1(x) = -x \\
\varphi_2(x) = x - 1.
\]

In this case

\[
U = \{x \in \mathbb{R} \mid -x \leq 0, x - 1 \leq 0\} = [0, 1].
\]

Since the constraints are affine, they are automatically qualified for any \(u \in [0, 1]\). The system of equations and inequalities shown above becomes

\[
1 - \lambda_1 + \lambda_2 = 0 \\
-\lambda_1 x + \lambda_2 (x - 1) = 0 \\
-x \leq 0 \\
x - 1 \leq 0 \\
\lambda_1, \lambda_2 \geq 0.
\]

The last four equations imply that either \(x = 0\) or \(x = 1\).

If \(x = 0\), by the second equation we get \(\lambda_2 = 0\), so \(\lambda_1 = 1 \geq 0\). Indeed \(x = 0\) is the minimum of \(J(x) = x\) over \([0, 1]\).

If \(x = 1\), by the second equation we get \(\lambda_1 = 0\), so \(\lambda_2 = -1\), a contradiction. Indeed, 1 is a maximum, and not a minimum of \(J(x) = x\) over \([0, 1]\).
14.2. THE KARUSH–KUHN–TUCKER CONDITIONS

Remark: Unless the linear forms \((\varphi'_i)_u\) for \(i \in I(u)\) are linearly independent, the \(\lambda_i(u)\) are generally not unique. Also, if \(I(u) = \emptyset\), then the KKT conditions reduce to \(J'_u = 0\). This is not surprising because in this case \(u\) belongs to the relative interior of \(U\).

If the constraints are all affine equality constraints, then the KKT conditions are a bit simpler. We will consider this case shortly.

The conditions for the qualification of nonaffine constraints are hard (if not impossible) to use in practice, because they depend on \(u \in U\) and on the derivatives \((\varphi'_i)_u\). Thus it is desirable to find simpler conditions. Fortunately, this is possible if the nonaffine functions \(\varphi_i\) are convex.

Definition 14.6. Let \(U \subseteq \Omega \subseteq V\) be given by

\[
U = \{x \in \Omega \mid \varphi_i(x) \leq 0, \ 1 \leq i \leq m\},
\]

where \(\Omega\) is an open subset of the Euclidean vector space \(V\). If the functions \(\varphi_i: \Omega \to \mathbb{R}\) are convex, we say that the constraints are qualified if the following conditions hold:

(a) Either the constraints \(\varphi_i\) are affine for all \(i = 1, \ldots, m\) and \(U \neq \emptyset\), or

(b) There is some vector \(v \in \Omega\) such that the following conditions hold for \(i = 1, \ldots, m\):

(i) \(\varphi_i(v) \leq 0\).

(ii) If \(\varphi_i\) is not affine, then \(\varphi_i(v) < 0\).

The above qualification conditions are known as Slater’s conditions.

Condition (b)(i) also implies that \(U\) has nonempty relative interior. If \(\Omega\) is convex, then \(U\) is also convex. This is because for all \(u, v \in \Omega\), if \(u \in U\) and \(v \in U\), that is \(\varphi_i(u) \leq 0\) and \(\varphi_i(v) \leq 0\) for \(i = 1, \ldots, m\), since the functions \(\varphi_i\) are convex, for all \(\theta \in [0, 1]\) we have

\[
\varphi_i((1 - \theta)u + \theta v) \leq (1 - \theta)\varphi_i(u) + \theta \varphi_i(v) \quad \text{since } \varphi_i \text{ is convex}
\]

\[
\leq 0 \quad \text{since } 1 - \theta \geq 0, \theta \geq 0, \varphi_i(u) \leq 0, \varphi_i(v) \leq 0,
\]

and any intersection of convex sets is convex.

It is important to observe that a nonaffine equality constraint \(\varphi_i(u) = 0\) is never qualified.

Indeed, \(\varphi_i(u) = 0\) is equivalent to \(\varphi_i(u) \leq 0\) and \(-\varphi_i(u) \leq 0\), so if these constraints are qualified and if \(\varphi_i\) is not affine then there is some nonzero vector \(v \in \Omega\) such that both \(\varphi_i(v) < 0\) and \(-\varphi_i(v) < 0\), which is impossible. For this reason, equality constraints are often assumed to be affine.

The following theorem yields a more flexible version of Theorem 31.5 for constraints given by convex functions. If in addition, the function \(J\) is also convex, then the KKT conditions are also a sufficient condition for a local minimum.
Theorem 14.6. Let $\varphi_i : \Omega \to \mathbb{R}$ be $m$ convex constraints defined on some open convex subset $\Omega$ of a finite-dimensional Euclidean vector space $V$ (more generally, a real Hilbert space $V$), let $J : \Omega \to \mathbb{R}$ be some function, let $U$ be given by

$$U = \{x \in \Omega \mid \varphi_i(x) \leq 0, \ 1 \leq i \leq m\},$$

and let $u \in U$ be any point such that the functions $\varphi_i$ and $J$ are differentiable at $u$.

(1) If $J$ has a local minimum at $u$ with respect to $U$, and if the constraints are qualified, then there exist some scalars $\lambda_i(u) \in \mathbb{R}$, such that the KKT condition hold:

$$J'_u + \sum_{i=1}^{m} \lambda_i(u) (\varphi'_i)_u = 0$$

and

$$\sum_{i=1}^{m} \lambda_i(u) \varphi_i(u) = 0, \quad \lambda_i(u) \geq 0, \quad i = 1, \ldots, m.$$

Equivalently, in terms of gradients, the above conditions are expressed as

$$\nabla J_u + \sum_{i=1}^{m} \lambda_i(u) \nabla (\varphi_i)_u = 0,$$

and

$$\sum_{i=1}^{m} \lambda_i(u) \varphi_i(u) = 0, \quad \lambda_i(u) \geq 0, \quad i = 1, \ldots, m.$$

(2) Conversely, if the restriction of $J$ to $U$ is convex and if there exist scalars $(\lambda_1, \ldots, \lambda_m) \in \mathbb{R}^m_+$ such that the KKT conditions hold, then the function $J$ has a (global) minimum at $u$ with respect to $U$.

Proof. (1) It suffices to prove that if the convex constraints are qualified according to Definition 31.6, then they are qualified according to Definition 31.5, since in this case we can apply Theorem 31.5.

If $v \in \Omega$ is a vector such that Condition (b) of Definition 31.6 holds and if $v \neq u$, for any $i \in I(u)$, since $\varphi_i(u) = 0$ and since $\varphi_i$ is convex, by Proposition 21.9,

$$\varphi_i(v) \geq \varphi_i(u) + (\varphi'_i)_u (v - u) = (\varphi'_i)_u (v - u),$$

so if we let $w = v - u$ then

$$(\varphi'_i)_u (w) \leq \varphi_i(v),$$

which shows that the nonaffine constraints $\varphi_i$ for $i \in I(u)$ are qualified according to Definition 31.5, by Condition (b) of Definition 31.6.
If \( v = u \), then the constraints \( \varphi_i \) for which \( \varphi_i(u) = 0 \) must be affine (otherwise, Condition (b)(ii) of Definition 31.6 would be false), and in this case we can pick \( w = 0 \).

(2) Let \( v \) be any arbitrary point in the convex subset \( U \). Since \( \varphi_i(v) \leq 0 \) and \( \lambda_i \geq 0 \) for \( i = 1, \ldots, m \), we have \( \sum_{i=1}^{m} \lambda_i \varphi_i(v) \leq 0 \), and using the fact that \( \sum_{i=1}^{m} \lambda_i \varphi_i(u) = 0 \), \( \lambda_i(u) \geq 0 \), \( i = 1, \ldots, m \), we have

\[
\lambda_i = 0 \text{ if } i \notin I(u) \quad \text{and} \quad \varphi_i(u) = 0 \text{ if } i \in I(u),
\]

so we have

\[
J(u) \leq J(u) - \sum_{i=1}^{m} \lambda_i \varphi_i(v)
\]

\[
\leq J(u) - \sum_{i \in I(u)} \lambda_i (\varphi_i(v) - \varphi_i(u)) \quad \lambda_i = 0 \text{ if } i \notin I(u), \varphi_i(u) = 0 \text{ if } i \in I(u)
\]

\[
\leq J(u) - \sum_{i \in I(u)} \lambda_i (\varphi'_i)_u (v - u) \quad \text{(by Proposition 21.9)}
\]

\[
\leq J(u) + J'_u (v - u) \quad \text{(by the KKT conditions)}
\]

\[
\leq J(v) \quad \text{(by Proposition 21.9)},
\]

and this shows that \( u \) is indeed a (global) minimum of \( J \) over \( U \). \( \square \)

It is important to note that when both the constraints, the domain of definition \( \Omega \), and the objective function \( J \) are convex, if the KKT conditions hold for some \( u \in U \) and some \( \lambda \in \mathbb{R}^m_+ \), then Theorem 31.6 implies that \( J \) has a (global) minimum at \( u \) with respect to \( U \), independently of any assumption on the qualification of the constraints.

The above theorem suggests introducing the function \( L: \Omega \times \mathbb{R}^m_+ \rightarrow \mathbb{R} \) given by

\[
L(v, \lambda) = J(v) + \sum_{i=1}^{m} \lambda_i \varphi_i(v),
\]

with \( \lambda = (\lambda_1, \ldots, \lambda_m) \). The function \( L \) is called the Lagrangian of the minimization problem (\( P \)):

\[
\text{minimize} \quad J(v) \\
\text{subject to} \quad \varphi_i(v) \leq 0, \quad i = 1, \ldots, m.
\]

The KKT conditions of Theorem 31.6 imply that for any \( u \in U \), if the vector \( \lambda = (\lambda_1, \ldots, \lambda_m) \) is known and if \( u \) is a minimum of \( J \) on \( U \), then

\[
\frac{\partial L}{\partial u}(u) = 0 \\
J(u) = L(u, \lambda).
\]
Chapter 14. Introduction to Nonlinear Optimization

The Lagrangian technique “absorbs” the constraints into the new objective function $L$ and reduces the problem of finding a constrained minimum of the function $J$, to the problem of finding an unconstrained minimum of the function $L(v, \lambda)$. This is the main point of Lagrangian duality which will be treated in the next section.

A case that arises often in practice is the case where the constraints $\varphi_i$ are affine. If so, the $m$ constraints $a_i x \leq b_i$ can be expressed in matrix form as $Ax \leq b$, where $A$ is an $m \times n$ matrix whose $i$th row is the row vector $a_i$. The KKT conditions of Theorem 31.6 yield the following corollary.

**Proposition 14.7.** If $U$ is given by

$$U = \{ x \in \Omega \mid Ax \leq b \},$$

where $\Omega$ is an open convex subset of $\mathbb{R}^n$ and $A$ is an $m \times n$ matrix, and if $J$ is differentiable at $u$ and $J$ has a local minimum at $u$, then there exist some vector $\lambda \in \mathbb{R}^m$, such that

$$\nabla J_u + A^\top \lambda = 0$$

$$\lambda_i \geq 0 \quad \text{and} \quad \text{if } a_i u < b_i \quad \text{then } \lambda_i = 0, \ i = 1, \ldots, m.$$  

If the function $J$ is convex, then the above conditions are also sufficient for $J$ to have a minimum at $u \in U$.

Another case of interest is the generalization of the minimization problem involving the affine constraints of a linear program in standard form, that is, equality constraints $Ax = b$ with $x \geq 0$, where $A$ is an $m \times n$ matrix. In our formalism, this corresponds to the $2m + n$ constraints

$$a_ix - b_i \leq 0, \quad i = 1, \ldots, m$$

$$-a_ix + b_i \leq 0, \quad i = 1, \ldots, m$$

$$-x_j \leq 0, \quad i = 1, \ldots, n.$$  

In matrix form, they can be expressed as

$$\begin{pmatrix}
A & -A & -I_n
\end{pmatrix}
\begin{pmatrix}
x_1 \\
\vdots \\
x_n
\end{pmatrix}
\leq
\begin{pmatrix}
b \\
-b \\
0_n
\end{pmatrix}.$$  

If we introduce the generalized Lagrange multipliers $\lambda_i^+$ and $\lambda_i^-$ for $i = 1, \ldots, m$ and $\mu_j$ for $j = 1, \ldots, n$, then the KKT conditions are

$$\nabla J_u + \begin{pmatrix} A^\top & -A^\top & -I_n \end{pmatrix} \begin{pmatrix} \lambda^+ \\ \lambda^- \\ \mu \end{pmatrix} = 0,$$
that is,

\[ \nabla J_u + A^T \lambda^+ - A^T \lambda^- - \mu = 0, \]

and \( \lambda^+, \lambda^-, \mu \geq 0 \), and if \( a_i u < b_i \) then \( \lambda^+_i = 0 \), if \( -a_i u < -b_i \) then \( \lambda^-_i = 0 \), and if \(-u_j < 0\), then \( \mu_j = 0 \). But the constraints \( a_i u = b_i \) hold for \( i = 1, \ldots, m \), so this places no restriction on the \( \lambda^+_i \) and \( \lambda^-_i \), and if we write \( \lambda_i = \lambda^+_i - \lambda^-_i \), then we have

\[ \nabla J_u + A^T \lambda = \mu, \]

with \( \mu_j \geq 0 \), and if \( u_j > 0 \) then \( \mu_j = 0 \), for \( j = 1, \ldots, n \).

Thus we proved the following proposition (which is slight generalization of Proposition 8.7.2 in Matousek and Gardner [73]).

**Proposition 14.8.** If \( U \) is given by

\[ U = \{ x \in \Omega \mid Ax = b, \ x \geq 0 \}, \]

where where \( \Omega \) is an open convex subset of \( \mathbb{R}^n \) and \( A \) is an \( m \times n \) matrix, and if \( J \) is differentiable at \( u \) and \( J \) has a local minimum at \( u \), then there exist two vectors \( \lambda \in \mathbb{R}^m \) \( \mu \in \mathbb{R}^n \), such that

\[ \nabla J_u + A^T \lambda = \mu, \]

with \( \mu_j \geq 0 \), and if \( u_j > 0 \) then \( \mu_j = 0 \), for \( j = 1, \ldots, n \). Equivalently, there exists a vector \( \lambda \in \mathbb{R}^m \) such that

\[ (\nabla J_u)_j + (A^T)_j \lambda \begin{cases} = 0 & \text{if } u_j > 0 \\ \geq 0 & \text{if } u_j = 0, \end{cases} \]

where \( A^T \) is the \( j \)th column of \( A \). If the function \( J \) is convex, then the above conditions are also sufficient for \( J \) to have a minimum at \( u \in U \).

Yet another special case that arises frequently in practice is the minimization problem involving the affine equality constraints \( Ax = b \), where \( A \) is an \( m \times n \) matrix, with no restriction on \( x \). Reviewing the proof of Proposition 31.8, we obtain the following proposition.

**Proposition 14.9.** If \( U \) is given by

\[ U = \{ x \in \Omega \mid Ax = b \}, \]

where \( \Omega \) is an open convex subset of \( \mathbb{R}^n \) and \( A \) is an \( m \times n \) matrix, and if \( J \) is differentiable at \( u \) and \( J \) has a local minimum at \( u \), then there exist some vector \( \lambda \in \mathbb{R}^m \) such that

\[ \nabla J_u + A^T \lambda = 0. \]

Equivalently, there exists a vector \( \lambda \in \mathbb{R}^m \) such that

\[ (\nabla J_u)_j + (A^T)_j \lambda = 0, \]

where \( A^T \) is the \( j \)th column of \( A \). If the function \( J \) is convex, then the above conditions are also sufficient for \( J \) to have a minimum at \( u \in U \).
Observe that in Proposition 31.9, the $\lambda_i$ are just standard Lagrange multipliers, with no restriction of positivity. Thus, Proposition 31.9 is a slight generalization of Theorem 21.3 that requires $A$ to have rank $m$, but in the case of equational affine constraints, this assumption is unnecessary.

Here is an application of Proposition 31.9 to the interior point method in linear programming.

**Example 14.4.** In linear programming, the interior point method using a central path uses a logarithmic barrier function to keep the solutions $x \in \mathbb{R}^n$ of the equation $Ax = b$ away from boundaries by forcing $x > 0$, which means that $x_i > 0$ for all $i$; see Matousek and Gardner [73] (Section 7.2). Write

$$\mathbb{R}^n_+ = \{ x \in \mathbb{R}^n \mid x_i > 0, \ i = 1, \ldots, n \}.$$ 

Observe that $\mathbb{R}^n_+$ is open and convex. For any $\mu > 0$, we define the function $f_\mu$ defined on $\mathbb{R}^n_+$ by

$$f_\mu(x) = c^\top x + \mu \sum_{i=1}^{n} \ln x_i,$$

where $c \in \mathbb{R}^n$.

We would like to find necessary condition for $f_\mu$ to have a maximum on

$$U = \{ x \in \mathbb{R}^n_+ \mid Ax = b \},$$

or equivalently to solve the following problem:

$$\begin{array}{ll}
\text{maximize} & f_\mu(x) \\
\text{subject to} & Ax = b \\
& x > 0.
\end{array}$$

By Proposition 31.9 if $x$ is an optimal of the above problem then there is some $y \in \mathbb{R}^n$ such that

$$\nabla f_\mu(x) + A^\top y = 0.$$

Since

$$\nabla f_\mu(x) = \begin{pmatrix} c_1 + \frac{\mu}{x_1} \\ \vdots \\ c_n + \frac{\mu}{x_n} \end{pmatrix},$$

we obtain the equation

$$c + \mu \begin{pmatrix} \frac{1}{x_1} \\ \vdots \\ \frac{1}{x_n} \end{pmatrix} = -A^\top y.$$
To obtain a more convenient formulation, we define $s \in \mathbb{R}^n_{++}$ such that

$$s = \mu \begin{pmatrix} \frac{1}{x_1} \\ \vdots \\ \frac{1}{x_n} \end{pmatrix}$$

which implies that

$$\begin{pmatrix} s_1 x_1 & \cdots & s_n x_n \end{pmatrix} = \mu \mathbf{1}_n^\top,$$

we rename $-y$ as $y$ (which does not make any difference since $y \in \mathbb{R}^m$), and we obtain the following necessary conditions for $f_\mu$ to have a maximum:

$$Ax = b$$
$$A^\top y - s = c$$
$$\begin{pmatrix} s_1 x_1 & \cdots & s_n x_n \end{pmatrix} = \mu \mathbf{1}_n^\top$$
$$s, x > 0.$$

It is not hard to show that if the primal linear program with objective function $c^\top x$ and equational constraints $Ax = b$ and the dual program with objective function $b^\top y$ and inequality constraints $A^\top y \geq c$ have interior feasible points $x$ and $y$, which means that $x > 0$ and $s > 0$ (where $s = A^\top y - c$), then the above system of equations has a unique solution such that $x$ is the unique maximizer of $f_\mu$ on $U$; see Matousek and Gardner [73] (Section 7.2, Lemma 7.2.1).

We now give an example illustrating Proposition 31.7, the Support Vector Machine (abbreviated as SVM).

### 14.3 Hard Margin Support Vector Machine; Version I

In this section we describe the following classification problem, or perhaps more accurately, separation problem (into two classes). Suppose we have two nonempty disjoint finite sets of $p$ blue points $\{u_i\}_{i=1}^p$ and $q$ red points $\{v_j\}_{j=1}^q$ in $\mathbb{R}^n$ (for simplicity, you may assume that these points are in the plane, that is, $n = 2$). Our goal is to find a hyperplane $H$ of equation $w^\top x - b = 0$ (where $w \in \mathbb{R}^n$ is a nonzero vector and $b \in \mathbb{R}$), such that all the blue points $u_i$ are in one of the two open half-spaces determined by $H$, and all the red points $v_j$ are in the other open half-space determined by $H$; see Figure 31.11.

Without loss of generality, we may assume that

$$w^\top u_i - b > 0 \quad \text{for } i = 1, \ldots, p$$
$$w^\top v_j - b < 0 \quad \text{for } j = 1, \ldots, q.$$
Figure 14.11: Two examples of the SVM separation problem. The left figure is SVM in $\mathbb{R}^2$, while the right figure is SVM in $\mathbb{R}^3$.

Of course, separating the blue and the red points may be impossible, as we see in Figure 31.12 for four points where the line segments $(u_1, u_2)$ and $(v_1, v_2)$ intersect. If a hyperplane separating the two subsets of blue and red points exists, we say that they are \textit{linearly separable}.

\textbf{Remark:} Write $m = p + q$. The reader should be aware that in machine learning the classification problem is usually defined as follows. We assign $m$ so-called class labels $y_k = \pm 1$ to the data points in such a way that $y_i = +1$ for each blue point $u_i$, and $y_{p+j} = -1$ for each red point $v_j$, and we denote the $m$ points by $x_k$, where $x_k = u_k$ for $k = 1, \ldots, p$ and $x_k = v_{k-p}$ for $k = p+1, \ldots, p+q$. Then the classification constraints can be written as

$$y_k (w^T x_k - b) > 0 \quad \text{for } k = 1, \ldots, m.$$ 

The set of pairs $\{(x_1, y_1), \ldots, (x_m, y_m)\}$ is called a set of \textit{training data} (or \textit{training set}).

In the sequel, we will not use the above method, and we will stick to our two subsets of $p$ \textit{blue} points $\{u_i\}_{i=1}^p$ and $q$ \textit{red} points $\{v_j\}_{j=1}^q$.

Since there are infinitely many hyperplanes separating the two subsets (if indeed the two subsets are linearly separable), we would like to come up with a “good” criterion for choosing such a hyperplane.

The idea that was advocated by Vapnik (see Vapnik [111]) is to consider the distances $d(u_i, H)$ and $d(v_j, H)$ from all the points to the hyperplane $H$, and to pick a hyperplane $H$ that maximizes the smallest of these distances. In machine learning this strategy is called finding a \textit{maximal margin hyperplane}, or \textit{hard margin support vector machine}, which definitely sounds more impressive.
Figure 14.12: Two examples in which it is impossible to find purple hyperplanes which separate the red and blue points.

Since the distance from a point $x$ to the hyperplane $H$ of equation $w^\top x - b = 0$ is

$$d(x, H) = \frac{|w^\top x - b|}{\|w\|},$$

(where $\|w\| = \sqrt{w^\top w}$ is the Euclidean norm of $w$), it is convenient to temporarily assume that $\|w\| = 1$, so that

$$d(x, H) = |w^\top x - b|.$$

See Figure 31.13. Then with our sign convention, we have

$$d(u_i, H) = w^\top u_i - b$$
$$d(v_j, H) = -w^\top v_j + b$$

If we let

$$\delta = \min\{d(u_i, H), d(v_j, H) \mid 1 \leq i \leq p, 1 \leq j \leq q\},$$

then the hyperplane $H$ should chosen so that

$$w^\top u_i - b \geq \delta$$
$$-w^\top v_j + b \geq \delta$$

and such that $\delta > 0$ is maximal. The distance $\delta$ is called the margin associated with the hyperplane $H$. This is indeed one way of formulating the two-class separation problem as an
optimization problem with a linear objective function \( J(\delta, w, b) = \delta \), and affine and quadratic constraints (SVM\(_h_1\)):

\[
\begin{align*}
\text{maximize} \quad & \delta \\
\text{subject to} \quad & w^\top u_i - b \geq \delta \quad i = 1, \ldots, p \\
\quad & -w^\top v_j + b \geq \delta \quad j = 1, \ldots, q \\
\quad & \|w\| \leq 1.
\end{align*}
\]

Observe that the Problem (SVM\(_{h_1}\)) has an optimal solution \( \delta > 0 \) iff the two subsets are linearly separable. We used the constraint \( \|w\| \leq 1 \) rather than \( \|w\| = 1 \) because the former is qualified, whereas the latter is not.

Actually, if \( (w, b, \delta) \) is an optimal solution of Problem (SVM\(_{h_1}\)), so in particular \( \delta > 0 \), then we claim that we must have \( \|w\| = 1 \). First, if \( w = 0 \), then we get the two inequalities

\[-b \geq \delta, \quad b \geq \delta,
\]

which imply that \( b \leq -\delta \) and \( b \geq \delta \) for some positive \( \delta \), which is impossible. But then, if \( w \neq 0 \) and \( \|w\| < 1 \), by dividing both sides of the inequalities by \( \|w\| < 1 \) we would obtain the better solution \( (w/\|w\|, b/\|w\|, \delta/\|w\|) \), since \( \|w\| < 1 \) implies that \( \delta/\|w\| > \delta \).

We now prove that if the two subsets are linearly separable, then Problem (SVM\(_{h_1}\)) has a unique optimal solution.

**Theorem 14.10.** If two disjoint subsets of \( p \) blue points \( \{u_i\}_{i=1}^p \) and \( q \) red points \( \{v_j\}_{j=1}^q \) are linearly separable, then Problem (SVM\(_{h_1}\)) has a unique optimal solution consisting of a
14.3. HARD MARGIN SUPPORT VECTOR MACHINE; VERSION I

hyperplane of equation \( w^\top x - b = 0 \) separating the two subsets with maximum margin \( \delta \). Furthermore, if we define \( c_1(w) \) and \( c_2(w) \) by

\[
\begin{align*}
  c_1(w) &= \min_{1 \leq i \leq p} w^\top u_i, \\
  c_2(w) &= \max_{1 \leq j \leq q} w^\top v_j,
\end{align*}
\]

then \( w \) is the unique maximum of the function

\[
\rho(w) = \frac{c_1(w) - c_2(w)}{2}
\]

over the convex subset \( U \) of \( \mathbb{R}^n \) given by the inequalities

\[
\begin{align*}
  w^\top u_i - b &\geq \delta & i = 1, \ldots, p \\
  -w^\top v_j + b &\geq \delta & j = 1, \ldots, q \\
  \|w\| &\leq 1,
\end{align*}
\]

and

\[
b = \frac{c_1(w) + c_2(w)}{2}.
\]

Proof. Our proof is adapted from Vapnik [111] (Chapter 10, Theorem 10.1). For any separating hyperplane \( H \), since

\[
\begin{align*}
  d(u_i, H) &= w^\top u_i - b & i = 1, \ldots, p \\
  d(v_j, H) &= -w^\top v_j + b & j = 1, \ldots, q,
\end{align*}
\]

and since the smallest distance to \( H \) is

\[
\delta = \min\{d(u_i, H), d(v_j, H) \mid 1 \leq i \leq p, 1 \leq j \leq q\}
= \min\{w^\top u_i - b, -w^\top v_j + b \mid 1 \leq i \leq p, 1 \leq j \leq q\}
= \min\{\min\{w^\top u_i - b \mid 1 \leq i \leq p\}, \min\{-w^\top v_j + b \mid 1 \leq j \leq q\}\}
= \min\{\min\{w^\top u_i \mid 1 \leq i \leq p\} - b, \min\{-w^\top v_j \mid 1 \leq j \leq q\} + b\}
= \min\{\min\{w^\top u_i \mid 1 \leq i \leq p\} - b\}, -\max\{-w^\top v_j \mid 1 \leq j \leq q\} + b\}
= \min\{c_1(w) - b, -c_2(w) + b\},
\]

in order for \( \delta \) to be maximal we must have

\[
c_1(w) - b = -c_2(w) + b,
\]

which yields

\[
b = \frac{c_1(w) + c_2(w)}{2}.
\]
In this case,
\[ c_1(w) - b = \frac{c_1(w) - c_2(w)}{2} = -c_2(w) + b, \]
so the maximum margin \( \delta \) is indeed obtained when \( \rho(w) = (c_1(w) - c_2(w))/2 \) is maximal over \( U \). Conversely, it is easy to see that any hyperplane of equation \( w^\top x - b = 0 \) associated with a \( w \) maximizing \( \rho \) over \( U \) and \( b = (c_1(w) + c_2(w))/2 \) is an optimal solution.

It remains to show that an optimal separating hyperplane exists and is unique. Since the unit ball is compact, \( U \) is compact, and since the function \( w \mapsto \rho(w) \) is continuous, it achieves its maximum for some \( w_0 \) such that \( \|w_0\| \leq 1 \). Actually, we must have \( \|w_0\| = 1 \), since otherwise, by a familiar reasoning \( w_0/\|w_0\| \) would be an even better solution. Therefore, \( w_0 \) is on the boundary of \( U \). But \( \rho \) is a concave function (as an infimum of affine functions), so if it had two distinct maxima \( w_0 \) and \( w'_0 \) with \( \|w_0\| = \|w'_0\| = 1 \), these would be global maxima since \( U \) is also convex, so we would have \( \rho(w_0) = \rho(w'_0) \) and then \( \rho \) would also have the same value along the segment \( (w_0, w'_0) \) and in particular at \( (w_0 + w'_0)/2 \), an interior point of \( U \), a contradiction. \( \square \)

We can proceed with the above formulation (SVM\(_{h1}\)) but there is a way to reformulate the problem so that the constraints are all affine, which might be preferable since they will be automatically qualified.

### 14.4 Hard Margin Support Vector Machine; Version II

Since \( \delta > 0 \) (otherwise the data would not be separable into two disjoint sets), we can divide the affine constraints by \( \delta \) to obtain
\[
\begin{align*}
    w^\top u_i - b' &\geq 1 & i = 1, \ldots, p \\
    -w^\top v_j + b' &\geq 1 & j = 1, \ldots, q,
\end{align*}
\]
extcept that now, \( w' \) is not necessarily a unit vector. To obtain the distances to the hyperplane \( H \), we need to divide by \( \|w'\| \) and then we have
\[
\begin{align*}
    \frac{w'^\top u_i - b'}{\|w'\|} &\geq \frac{1}{\|w'\|} & i = 1, \ldots, p \\
    \frac{-w'^\top v_j + b'}{\|w'\|} &\geq \frac{1}{\|w'\|} & j = 1, \ldots, q,
\end{align*}
\]
which means that the shortest distance from the data points to the hyperplane is \( 1/\|w'\| \). Therefore, we wish to maximize \( 1/\|w'\| \), that is, to minimize \( \|w'\| \), so we obtain the following optimization problem (SVM\(_{h2}\)):
14.4. HARD MARGIN SUPPORT VECTOR MACHINE; VERSION II

**Hard margin SVM (SVM\textsubscript{h2}):**

\[
\begin{align*}
\text{minimize} & \quad \frac{1}{2} \|w\|^2 \\
\text{subject to} & \quad w^\top u_i - b \geq 1 \quad i = 1, \ldots, p \\
& \quad -w^\top v_j + b \geq 1 \quad j = 1, \ldots, q.
\end{align*}
\]

The objective function \( J(w) = \frac{1}{2} \|w\|^2 \) is convex, so Proposition 31.7 applies and gives us a necessary and sufficient condition for having a minimum in terms of the KKT conditions. First observe that the trivial solution \( w = 0 \) is impossible, because the blue constraints would be

\[-b \geq 1,
\]

that is \( b \leq -1 \), and the red constraints would be

\[b \geq 1,
\]

but these are contradictory. Our goal is to find \( w \) and \( b \), and optionally, \( \delta \). We proceed in four steps first demonstrated on the following example.

Suppose that \( p = q = n = 2 \), so that we have two blue points

\[w_1^\top = (u_{11}, u_{12}) \quad w_2^\top = (u_{21}, u_{22}),
\]

two red points

\[v_1^\top = (v_{11}, v_{12}) \quad v_2^\top = (v_{21}, v_{22}),
\]

and\n
\[w^\top = (w_1, w_2).
\]

**Step 1:** Write the constraints in matrix form. Let

\[C = \begin{pmatrix}
-u_{11} & -u_{12} & 1 \\
-u_{21} & -u_{22} & 1 \\
v_{11} & v_{12} & -1 \\
v_{21} & v_{22} & -1
\end{pmatrix}, \quad d = \begin{pmatrix}
-1 \\
-1 \\
-1 \\
-1
\end{pmatrix}.
\]

\[(M)\]

The constraints become

\[C \begin{pmatrix} w \\ b \end{pmatrix} = \begin{pmatrix}
-u_{11} & -u_{12} & 1 \\
-u_{21} & -u_{22} & 1 \\
v_{11} & v_{12} & -1 \\
v_{21} & v_{22} & -1
\end{pmatrix} \begin{pmatrix} w_1 \\ w_2 \\ b \end{pmatrix} \leq \begin{pmatrix}
-1 \\
-1 \\
-1 \\
-1
\end{pmatrix}.
\]

\[(C)\]
**Step 2:** Write the objective function in matrix form.

\[
J(w_1, w_2, b) = \frac{1}{2} \begin{pmatrix} w_1 & w_2 & b \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} w_1 \\ w_2 \\ b \end{pmatrix}.
\]

\((O)\)

**Step 3:** Apply Proposition 31.7 to solve for \(w\) in terms of \(\lambda\) and \(\mu\). We obtain

\[
\begin{pmatrix} w_1 \\ w_2 \\ 0 \end{pmatrix} + \begin{pmatrix} -u_{11} & -u_{21} & v_{11} & v_{21} \\ -u_{12} & -u_{22} & v_{12} & v_{22} \\ 1 & 1 & -1 & -1 \end{pmatrix} \begin{pmatrix} \lambda_1 \\ \lambda_2 \\ \mu_1 \\ \mu_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix},
\]

i.e.

\[
\nabla J_{(w,b)} + C^\top \begin{pmatrix} \lambda \\ \mu \end{pmatrix} = 0_{n+1}.
\]

Then

\[
\begin{pmatrix} w_1 \\ w_2 \\ 0 \end{pmatrix} = \begin{pmatrix} u_{11} & u_{21} & -v_{11} & -v_{21} \\ u_{12} & u_{22} & -v_{12} & -v_{22} \\ -1 & -1 & 1 & 1 \end{pmatrix} \begin{pmatrix} \lambda_1 \\ \lambda_2 \\ \mu_1 \\ \mu_2 \end{pmatrix},
\]

which implies

\[
w = \begin{pmatrix} w_1 \\ w_2 \end{pmatrix} = \lambda_1 \begin{pmatrix} u_{11} \\ u_{12} \end{pmatrix} + \lambda_2 \begin{pmatrix} u_{21} \\ u_{22} \end{pmatrix} - \mu_1 \begin{pmatrix} v_{11} \\ v_{12} \end{pmatrix} - \mu_2 \begin{pmatrix} v_{21} \\ v_{22} \end{pmatrix} \quad \text{(*)}
\]

with respect to

\[
\mu_1 + \mu_2 - \lambda_1 - \lambda_2 = 0. \quad \text{(**)}
\]

**Step 4:** Rewrite the constraints at \((C)\) using \((*)\). In particular \(C \begin{pmatrix} w \\ b \end{pmatrix} \leq d\) becomes

\[
\begin{pmatrix} -u_{11} & -u_{12} & 1 \\ -u_{21} & -u_{22} & 1 \\ u_{11} & v_{11} & -1 \\ v_{12} & v_{11} & -1 \\ v_{21} & v_{22} & -1 \end{pmatrix} \begin{pmatrix} u_{11} & u_{21} & -v_{11} & -v_{21} & 0 \\ u_{12} & u_{22} & -v_{12} & -v_{22} & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \lambda_1 \\ \lambda_2 \\ \mu_1 \\ \mu_2 \end{pmatrix} \leq \begin{pmatrix} -1 \\ -1 \\ -1 \\ -1 \end{pmatrix}.
\]

Rewriting the previous equation in “block” format gives us

\[
-\begin{pmatrix} -u_{11} & -u_{12} \\ -u_{21} & -u_{22} \\ v_{11} & v_{12} \\ v_{21} & v_{22} \end{pmatrix} \begin{pmatrix} -u_{11} & -u_{21} & v_{11} & v_{21} \\ -u_{12} & -u_{22} & v_{21} & v_{22} \end{pmatrix} \begin{pmatrix} \lambda_1 \\ \lambda_2 \\ \mu_1 \\ \mu_2 \end{pmatrix} + b \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} \leq \begin{pmatrix} 0 \\ 0 \end{pmatrix},
\]
which with the definition
\[ X = \begin{pmatrix} -u_{11} & -u_{21} & v_{11} & v_{21} \\ -u_{12} & -u_{22} & v_{21} & v_{22} \end{pmatrix} \]
yields
\[ -X^{\top}X \begin{pmatrix} \lambda \\ \mu \end{pmatrix} + b \begin{pmatrix} 1_p \\ -1_q \end{pmatrix} + 1_{p+q} \leq 0_{p+q}. \] (*)

Let us now consider the general case.

**Step 1:** Write the constraints in matrix form. First we rewrite the constraints as
\[-u_i^{\top}w + b \leq -1 \quad \text{for } i = 1, \ldots, p\]
\[v_j^{\top}w - b \leq -1 \quad \text{for } j = 1, \ldots, q,\]
and we get the \((p + q) \times (n + 1)\) matrix \(C\) and the vector \(d \in \mathbb{R}^{p+q}\) given by
\[ C = \begin{pmatrix} -u_1^{\top} & 1 & \vdots & \vdots \\ -u_p^{\top} & 1 & \vdots & \vdots \\ v_1 & -1 & \vdots & \vdots \\ v_q & -1 \end{pmatrix}, \quad d = \begin{pmatrix} -1 \\ \vdots \\ -1 \end{pmatrix}, \]
so the set of inequality constraints is
\[ C \begin{pmatrix} w \\ b \end{pmatrix} \leq d. \]

**Step 2:** The objective function in matrix form is given by
\[ J(w, b) = \frac{1}{2} \begin{pmatrix} w^{\top} & b \end{pmatrix} \begin{pmatrix} I_n & 0_n \\ 0_n^{\top} & 0 \end{pmatrix} \begin{pmatrix} w \\ b \end{pmatrix}. \]
Note that the corresponding matrix is symmetric positive semidefinite, but it is *not* invertible. Thus the function \(J\) is convex but not strictly convex. This will cause some minor trouble in finding the dual function of the problem.

**Step 3:** If we introduce the generalized Lagrange multipliers \(\lambda \in \mathbb{R}^p\) and \(\mu \in \mathbb{R}^q\), according to Proposition 31.7, the first KKT condition is
\[ \nabla J_{(w,b)} + C^{\top} \begin{pmatrix} \lambda \\ \mu \end{pmatrix} = 0_{n+1}, \]
with \(\lambda \geq 0, \mu \geq 0\). By the result of Example 20.4,
\[ \nabla J_{(w,b)} = \begin{pmatrix} I_n & 0_n \\ 0_n^{\top} & 0 \end{pmatrix} \begin{pmatrix} w \\ b \end{pmatrix} = \begin{pmatrix} w \\ 0 \end{pmatrix}. \]
so we get
\[
\begin{pmatrix}
w \\
0
\end{pmatrix} = -C^\top \begin{pmatrix}
\lambda \\
\mu
\end{pmatrix},
\]
that is,
\[
\begin{pmatrix}
w \\
0
\end{pmatrix} = \begin{pmatrix}
u_1 & \cdots & u_p & -v_1 & \cdots & -v_q \\
-1 & \cdots & -1 & 1 & \cdots & 1
\end{pmatrix} \begin{pmatrix}
\lambda \\
\mu
\end{pmatrix}.
\]
Consequently,
\[
w = \sum_{i=1}^{p} \lambda_i u_i - \sum_{j=1}^{q} \mu_j v_j,
\]
and
\[
\sum_{j=1}^{q} \mu_j - \sum_{i=1}^{p} \lambda_i = 0.
\]

**Step 4:** Rewrite the constraints using \((\ast_1)\). Plugging the above expression for \(w\) into the constraints \(C \begin{pmatrix} w \\ b \end{pmatrix} \leq d\) we get
\[
\begin{pmatrix}
-u_1^\top & 1 \\
\vdots & \vdots \\
-u_p^\top & 1 \\
v_1^\top & -1 \\
\vdots & \vdots \\
v_q^\top & -1
\end{pmatrix}
\begin{pmatrix}
u_1 & \cdots & u_p & -v_1 & \cdots & -v_q & 0_n \\
0 & \cdots & 0 & 0 & \cdots & 0 & 1
\end{pmatrix}
\begin{pmatrix}
\lambda \\
\mu
\end{pmatrix} \leq \begin{pmatrix}
-1 \\
\vdots \\
-1
\end{pmatrix},
\]
so if let \(X\) be the \(n \times (p + q)\) matrix given by
\[
X = \begin{pmatrix}
-u_1 & \cdots & -u_p & v_1 & \cdots & v_q
\end{pmatrix},
\]
we obtain
\[
w = -X \begin{pmatrix}
\lambda \\
\mu
\end{pmatrix},
\]
and the above inequalities are written in matrix form as
\[
\begin{pmatrix}
X^\top & 1_p \\
-1_q^-1_p
\end{pmatrix}
\begin{pmatrix}
-X & 0_n \\
0_{p+q} & 1
\end{pmatrix}
\begin{pmatrix}
\lambda \\
\mu
\end{pmatrix} \leq -1_{p+q};
\]
that is,
\[
-X^\top X \begin{pmatrix}
\lambda \\
\mu
\end{pmatrix} + b \left(1_p \begin{pmatrix} 1_q^-1_p \end{pmatrix} + 1_{p+q} \right) \leq 0_{p+q}.
\]
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Equivalently, the $i$th inequality is

$$- \sum_{j=1}^{p} u_i^T u_j \lambda_j + \sum_{k=1}^{q} u_i^T v_k \mu_k + b + 1 \leq 0 \quad i = 1, \ldots, p,$$

and the $(p + j)$th inequality is

$$\sum_{i=1}^{p} v_j^T u_i \lambda_i - \sum_{k=1}^{q} v_j^T v_k \mu_k - b + 1 \leq 0 \quad j = 1, \ldots, q.$$

We also have $\lambda \geq 0, \mu \geq 0$. Furthermore, if the $i$th inequality is inactive then $\lambda_i = 0$, and if the $(p + j)$th inequality is inactive then $\mu_j = 0$. Since the constraints are affine and since $J$ is convex, if we can find $\lambda \geq 0, \mu \geq 0, b$ such that the inequalities in $(\ast_3)$ are satisfied, and $\lambda_i = 0$ and $\mu_j = 0$ when the corresponding constraint is inactive, then by Proposition 31.7 we have an optimum solution.

**Remark:** The second KKT condition can be written as

$$(\lambda^T \mu^T) \left(-X^T X \begin{pmatrix} \lambda \\ \mu \end{pmatrix} + b \begin{pmatrix} 1_p \\ -1_q \end{pmatrix} + 1_{p+q} \right) = 0;$$

that is,

$$- (\lambda^T \mu^T) X^T X \begin{pmatrix} \lambda \\ \mu \end{pmatrix} + b \left( \begin{pmatrix} 1_p \\ -1_q \end{pmatrix} \right) + (\lambda^T \mu^T) 1_{p+q} = 0.$$

Since $(\ast_2)$ says that $\sum_{i=1}^{p} \lambda_i = \sum_{j=1}^{q} \mu_j$, the second term is zero, and by $(\ast'_3)$ we get

$$w^T w = \begin{pmatrix} \lambda^T \\ \mu^T \end{pmatrix} X^T X \begin{pmatrix} \lambda \\ \mu \end{pmatrix} = \sum_{i=1}^{p} \lambda_i + \sum_{j=1}^{q} \mu_j.$$

Thus we obtain a simple expression for $\|w\|^2$ in terms of $\lambda$ and $\mu$.

The vectors $u_i$ and $v_j$ for which the $i$-th inequality is active and the $(p + j)$th inequality is active are called support vectors. For every vector $u_i$ or $v_j$ that is not a support vector, the corresponding inequality is inactive so $\lambda_i = 0$ and $\mu_j = 0$. Thus we see that only the support vectors contribute to a solution. If we can guess which vectors $u_i$ and $v_j$ are support vectors, namely, those for which $\lambda_i \neq 0$ and $\mu_j \neq 0$, then for each support vector $u_i$ we have an equation

$$- \sum_{j=1}^{p} u_i^T u_j \lambda_j + \sum_{k=1}^{q} u_i^T v_k \mu_k + b + 1 = 0,$$

and for each support vector $v_j$ we have an equation

$$\sum_{i=1}^{p} v_j^T u_i \lambda_i - \sum_{k=1}^{q} v_j^T v_k \mu_k - b + 1 = 0,$$
with $\lambda_i = 0$ and $\mu_j = 0$ for all non-support vectors, so together with the Equation $(*)_2$ we have a linear system with an equal number of equations and variables, which is solvable if our separation problem has a solution. Thus, in principle we can find $\lambda, \mu,$ and $b$ by solving a linear system.

**Remark:** We can first solve for $\lambda$ and $\mu$ (by eliminating $b$), and by $(*)_1$ and since $w \neq 0,$ there is at least some nonzero $\lambda_i_0$ and thus some nonzero $\mu_j_0,$ so the corresponding inequalities are equations

$$- \sum_{j=1}^p u_{i_0}^T u_j \lambda_j + \sum_{k=1}^q u_{i_0}^T v_k \mu_k + b + 1 = 0$$

$$\sum_{i=1}^p v_{j_0}^T u_i \lambda_i - \sum_{k=1}^q v_{j_0}^T v_k \mu_k - b + 1 = 0,$$

so $b$ is given in terms of $\lambda$ and $\mu$ by

$$b = \frac{1}{2} (u_{i_0}^T + v_{j_0}^T) \left( \sum_{i=1}^p \lambda_i u_i - \sum_{j=1}^p \mu_j v_j \right).$$

Using the dual of the Lagrangian, we can solve for $\lambda$ and $\mu,$ but typically $b$ is not determined, so we use the above method to find $b.$

The above nondeterministic procedure in which we guess which vectors are support vectors is not practical. We will see later that a practical method for solving for $\lambda$ and $\mu$ consists in maximizing the dual of the Lagrangian.

If $w$ is an optimal solution, then $\delta = 1/\|w\|$ is the shortest distance from the support vectors to the separating hyperplane $H_{w,b}$ of equation $w^T x - b = 0.$ If we consider the two hyperplanes $H_{w,b+1}$ and $H_{w,b-1}$ of equations

$$w^T x - b - 1 = 0 \quad \text{and} \quad w^T x - b + 1 = 0,$$

then $H_{w,b+1}$ and $H_{w,b-1}$ are two hyperplanes parallel to the hyperplane $H_{w,b}$ and the distance between them is $2\delta.$ Furthermore, $H_{w,b+1}$ contains the support vectors $u_i,$ $H_{w,b-1}$ contains the support vectors $v_j,$ and there are no data points $u_i$ or $v_j$ in the open region between these two hyperplanes containing the separating hyperplane $H_{w,b}$ (called a “slab” by Boyd and Vandenberghe; see [22], Section 8.6). This situation is illustrated in Figure 31.14.

Even if $p = 1$ and $q = 2,$ a solution is not obvious. In the plane, there are four possibilities:

(1) If $u_1$ is on the segment $(v_1, v_2),$ there is no solution.

(2) If the projection $h$ of $u_1$ onto the line determined by $v_1$ and $v_2$ is between $v_1$ and $v_2,$ that is $h = (1 - \alpha)v_1 + \alpha v_2$ with $0 \leq \alpha \leq 1,$ then it is the line parallel to $v_2 - v_1$ and equidistant to $u$ and both $v_1$ and $v_2,$ as illustrated in Figure 31.15.
Figure 14.14: In $\mathbb{R}^3$, the solution to the hard margin SVM is the purple plane sandwiched between the red plane $w^\top x - b + 1 = 0$ and the blue plane $w^\top x - b - 1 = 0$, each of which contains the appropriate support vectors $u_i$ and $v_j$.

(3) If the projection $h$ of $u_1$ onto the line determined by $v_1$ and $v_2$ is to the right of $v_2$, that is $h = (1 - \alpha)v_1 + \alpha v_2$ with $\alpha > 1$, then it is the bisector of the line segment $(u_1, v_2)$.

(4) If the projection $h$ of $u_1$ onto the line determined by $v_1$ and $v_2$ is to the left of $v_1$, that is $h = (1 - \alpha)v_1 + \alpha v_2$ with $\alpha < 0$, then it is the bisector of the line segment $(u_1, v_1)$.

If $p = q = 1$, we can find a solution explicitly. Then $(\ast_2)$ yields

$$\lambda = \mu,$$

and if we guess that the constraints are active, the corresponding equality constraints are

$$-u^\top u\lambda + u^\top v\mu + b + 1 = 0$$

$$u^\top v\lambda - v^\top v\mu - b + 1 = 0,$$

so we get

$$(-u^\top u + u^\top v)\lambda + b + 1 = 0$$

$$(u^\top v - v^\top v)\lambda - b + 1 = 0,$$

Adding up the two equations we find

$$(2u^\top v - u^\top u - v^\top v)\lambda + 2 = 0,$$
that is
\[ \lambda = \frac{2}{(u - v)\top(u - v)}. \]
By subtracting the first equation from the second, we find
\[ (u\top u - v\top v)\lambda - 2b = 0, \]
which yields
\[ b = \lambda \frac{(u\top u - v\top v)}{2} = \frac{u\top u - v\top v}{(u - v)\top(u - v)}. \]
Then by (\text{*}_1) we obtain
\[ w = \frac{2(u - v)}{(u - v)\top(u - v)}. \]
We verify easily that
\[ 2(u_1 - v_1)x_1 + \cdots + 2(u_n - v_n)x_n = (u_1^2 + \cdots + u_n^2) - (v_1^2 + \cdots + v_n^2) \]
is the equation of the bisector hyperplane between \( u \) and \( v \); see Figure 31.16.

In the next section we will derive the dual of the optimization problem discussed in this section. We will also consider a more flexible solution involving a soft margin.

### 14.5 Lagrangian Duality and Saddle Points

In this section we investigate methods to solve the minimization problem \((P)\):

\[
\begin{align*}
\text{minimize} & \quad J(v) \\
\text{subject to} & \quad \varphi_i(v) \leq 0, \quad i = 1, \ldots, m.
\end{align*}
\]
It turns out that under certain conditions the original problem \((P)\), called primal problem, can be solved in two stages with the help another problem \((D)\), called the dual problem. The dual problem \((D)\) is a maximization problem involving a function \(G\), called the Lagrangian dual, and it is obtained by minimizing the Lagrangian \(L(v, \mu)\) of Problem \((P)\) over the variable \(v \in \mathbb{R}^n\), holding \(\mu\) fixed, where \(L: \Omega \times \mathbb{R}_+^m \to \mathbb{R}\) is given by

\[
L(v, \mu) = J(v) + \sum_{i=1}^{m} \mu_i \varphi_i(v),
\]

with \(\mu \in \mathbb{R}_+^m\).

The two steps of the method are:

1. Find the dual function \(\mu \mapsto G(\mu)\) explicitly by solving the minimization problem of finding the minimum of \(L(v, \mu)\) with respect to \(v \in \Omega\), holding \(\mu\) fixed. This is an unconstrained minimization problem (with \(v \in \Omega\)). If we are lucky, a unique minimizer \(u_\mu\) such that \(G(\mu) = L(u_\mu, \mu)\) can be found. We will address the issue of uniqueness later on.

2. Solve the maximization problem of finding the maximum of the function \(\mu \mapsto G(\mu)\) over all \(\mu \in \mathbb{R}_+^m\). This is basically an unconstrained problem, except for the fact that \(\mu \in \mathbb{R}_+^m\).

If steps (1) and (2) are successful, under some suitable conditions on the function \(J\) and the constraints \(\varphi_i\) (for example, if they are convex), for any solution \(\lambda \in \mathbb{R}_+^m\) obtained in
step (2), the vector \( u_\lambda \) obtained in step (1) is an optimal solution of Problem \((P)\). This is proved in Theorem 31.14.

In order to prove Theorem 31.14, which is our main result, we need two intermediate technical results of independent interest involving the notion of saddle point.

The local minima of a function \( J: \Omega \to \mathbb{R} \) over a domain \( U \) defined by inequality constraints are saddle points of the Lagrangian \( L(u, \mu) \) associated with \( J \) and the constraints \( \varphi_i \). Then, under some mild hypotheses, the set of solutions of the minimization problem \((P)\)

\[
\begin{align*}
\text{minimize} & \quad J(v) \\
\text{subject to} & \quad \varphi_i(v) \leq 0, \quad i = 1, \ldots, m
\end{align*}
\]

coincides with the set of first arguments of the saddle points of the Lagrangian

\[
L(v, \mu) = J(v) + \sum_{i=1}^{m} \mu_i \varphi_i(v).
\]

This is proved in Theorem 31.12. To prove Theorem 31.14, we also need Proposition 31.11, a basic property of saddle points.

**Definition 14.7.** Let \( L: \Omega \times M \to \mathbb{R} \) be a function defined on a set of the form \( \Omega \times M \). A point \((u, \lambda)\in \Omega \times M\) is a saddle point of \( L \) if \( u \) is a minimum of the function \( L(-, \lambda): \Omega \to \mathbb{R} \) given by \( v \mapsto L(v, \lambda) \) for all \( v \in \Omega \) and \( \lambda \) fixed, and \( \lambda \) is a maximum of the function \( L(u,-): M \to \mathbb{R} \) given by \( \mu \mapsto L(u, \mu) \) for all \( \mu \in M \) and \( u \) fixed; equivalently,

\[
\sup_{\mu \in M} L(u, \mu) = L(u, \lambda) = \inf_{v \in \Omega} L(v, \lambda).
\]

Note that the order of the arguments \( u \) and \( \lambda \) is important. The second set \( M \) will be the set of generalized multipliers, and this is why we use the symbol \( M \).

A saddle point is often depicted as a mountain pass, which explains the terminology; see Figure 31.17. However, this is a bit misleading since other situations are possible; see Figure 31.18.

**Proposition 14.11.** If \((u, \lambda)\) is a saddle point of a function \( L: \Omega \times M \to \mathbb{R} \), then

\[
\sup_{\mu \in M} \inf_{v \in \Omega} L(v, \mu) = L(u, \lambda) = \inf_{v \in \Omega} \sup_{\mu \in M} L(v, \mu).
\]

**Proof.** First we prove that the following inequality always holds:

\[
\sup_{\mu \in M} \inf_{v \in \Omega} L(v, \mu) \leq \inf_{v \in \Omega} \sup_{\mu \in M} L(v, \mu).
\]

\[\text{(*)}_1\]

Pick any \( w \in \Omega \) and any \( \rho \in M \). By definition of inf (the greatest lower bound) and sup (the least upper bound), we have

\[
\inf_{v \in \Omega} L(v, \rho) \leq L(w, \rho) \leq \sup_{\mu \in M} L(w, \mu).
\]
The cases where \( \inf_{v \in \Omega} L(v, \rho) = -\infty \) or where \( \sup_{\mu \in M} L(w, \mu) = +\infty \) may arise, but this is not a problem. Since

\[
\inf_{v \in \Omega} L(v, \rho) \leq \sup_{\mu \in M} L(w, \mu)
\]

and the right-hand side is independent of \( \rho \), it is an upper bound of the left-hand side for all \( \rho \), so

\[
\sup_{\mu \in M} \inf_{v \in \Omega} L(v, \mu) \leq \sup_{\mu \in M} L(w, \mu).
\]

Since the left-hand side is independent of \( w \), it is a lower bound for the right-hand side for all \( w \), so we obtain \((*)_1\):

\[
\sup_{\mu \in M} \inf_{v \in \Omega} L(v, \mu) \leq \inf_{v \in \Omega} \sup_{\mu \in M} L(v, \mu).
\]

To obtain the reverse inequality, we use the fact that \((\lambda, \mu)\) is a saddle point, so

\[
\inf_{v \in \Omega} \sup_{\mu \in M} L(v, \mu) \leq \sup_{\mu \in M} L(u, \mu) = L(u, \lambda)
\]

and

\[
L(u, \lambda) = \inf_{v \in \Omega} L(v, \lambda) \leq \sup_{\mu \in M} \inf_{v \in \Omega} L(v, \mu),
\]

and these imply that

\[
\inf_{v \in \Omega} \sup_{\mu \in M} L(v, \mu) \leq \sup_{\mu \in M} \inf_{v \in \Omega} L(v, \mu), \quad (*_2)
\]

as desired. \( \square \)
Figure 14.18: Let $\Omega = \{[t, 0, 0] \mid 0 \leq t \leq 1\}$ and $M = \{[0, t, 0] \mid 0 \leq t \leq 1\}$. In Figure (i.), $L(u, \lambda)$ is the blue slanted quadrilateral whose forward vertex is a saddle point. In Figure (ii.), $L(u, \lambda)$ is the planar green rectangle composed entirely of saddle points.

We now return to our main minimization problem $(P)$:

$$\begin{align*}
\text{minimize} & \quad J(v) \\
\text{subject to} & \quad \varphi_i(v) \leq 0, \quad i = 1, \ldots, m,
\end{align*}$$

where $J: \Omega \to \mathbb{R}$ and the constraints $\varphi_i: \Omega \to \mathbb{R}$ are some functions defined on some open subset $\Omega$ of some finite-dimensional Euclidean vector space $V$ (more generally, a real Hilbert space $V$).

**Definition 14.8.** The Lagrangian of the minimization problem $(P)$ defined above is the function $L: \Omega \times \mathbb{R}^m_+ \to \mathbb{R}$ given by

$$L(v, \mu) = J(v) + \sum_{i=1}^{m} \mu_i \varphi_i(v),$$
with \( \mu = (\mu_1, \ldots, \mu_m) \). The numbers \( \mu_i \) are called \textit{generalized Lagrange multipliers}.

The following theorem shows that under some suitable conditions, every solution \( u \) of the Problem \((P)\) is the first argument of a saddle point \((u, \lambda)\) of the Lagrangian \( L \), and conversely, if \((u, \lambda)\) is a saddle point of the Lagrangian \( L \), then \( u \) is a solution of the Problem \((P)\).

\textbf{Theorem 14.12.} Consider Problem \((P)\) defined above where \( J: \Omega \to \mathbb{R} \) and the constraints \( \varphi_i: \Omega \to \mathbb{R} \) are some functions defined on some open subset \( \Omega \) of some finite-dimensional Euclidean vector space \( V \) (more generally, a real Hilbert space \( V \)). The following facts hold.

(1) If \((u, \lambda) \in \Omega \times \mathbb{R}_+^m \) is a saddle point of the Lagrangian \( L \) associated with Problem \((P)\), then \( u \in U \), \( u \) is a solution of Problem \((P)\), and \( J(u) = L(u, \lambda) \).

(2) If \( \Omega \) is convex (open), if the functions \( \varphi_i \) \((1 \leq i \leq m)\) and \( J \) are convex and differentiable at the point \( u \in U \), if the constraints are qualified, and if \( u \in U \) is a minimum of Problem \((P)\), then there exists some vector \( \lambda \in \mathbb{R}_+^m \) such that the pair \((u, \lambda) \in \Omega \times \mathbb{R}_+^m \) is a saddle point of the Lagrangian \( L \).

\textit{Proof.} (1) Since \((u, \lambda)\) is a saddle point of \( L \) we have \( \sup_{\mu \in M} L(u, \mu) = L(u, \lambda) \) which implies that \( L(u, \mu) \leq L(u, \lambda) \) for all \( \mu \in \mathbb{R}_+^m \), which means that

\[
J(u) + \sum_{i=1}^{m} \mu_i \varphi_i(u) \leq J(u) + \sum_{i=1}^{m} \lambda_i \varphi_i(u),
\]

that is,

\[
\sum_{i=1}^{m} (\mu_i - \lambda_i) \varphi_i(u) \leq 0 \quad \text{for all} \quad \mu \in \mathbb{R}_+^m.
\]

If we let each \( \mu_i \) be large enough, then \( \mu_i - \lambda_i > 0 \), and if we had \( \varphi_i(u) > 0 \) then the term \( (\mu_i - \lambda_i) \varphi_i(u) \) could be made arbitrarily large and positive, so we conclude that \( \varphi_i(u) \leq 0 \) for \( i = 1, \ldots, m \), and consequently, \( u \in U \). For \( \mu = 0 \), we conclude that \( \sum_{i=1}^{m} \lambda_i \varphi_i(u) \geq 0 \), while since \( \lambda_i \geq 0 \) and \( \varphi_i(u) \leq 0 \) we have \( \sum_{i=1}^{m} \lambda_i \varphi_i(u) \leq 0 \), so we must have \( u \in U \) and

\[
\sum_{i=1}^{m} \lambda_i \varphi_i(u) = 0. \tag{\ast_1}
\]

This shows that \( J(u) = L(u, \lambda) \). Since the inequality \( L(u, \lambda) \leq L(v, \lambda) \) is

\[
J(u) + \sum_{i=1}^{m} \lambda_i \varphi_i(u) \leq J(v) + \sum_{i=1}^{m} \lambda_i \varphi_i(v),
\]

by \( \ast_1 \) we obtain

\[
J(u) \leq J(v) + \sum_{i=1}^{m} \lambda_i \varphi_i(v) \quad \text{for all} \quad v \in \Omega
\]

\[
\leq J(v) \quad \text{for all} \quad v \in U \quad \text{(since} \quad \varphi_i(v) \leq 0 \text{ and} \quad \lambda_i \geq 0),
\]
which shows that \( u \) is a minimum of \( J \) on \( U \).

(2) The hypotheses required to apply Theorem 31.6(1) are satisfied. Consequently if \( u \in U \) is a solution of Problem \((P)\), then there exists some vector \( \lambda \in \mathbb{R}_+^m \) such that the KKT conditions hold:

\[
J'(u) + \sum_{i=1}^m \lambda_i \varphi'_i(u) = 0 \quad \text{and} \quad \sum_{i=1}^m \lambda_i \varphi_i(u) = 0.
\]

The second equation yields

\[
L(u, \mu) = J(u) + \sum_{i=1}^m \mu_i \varphi_i(u) \leq J(u) = J(u) + \sum_{i=1}^m \lambda_i \varphi_i(u) = L(u, \lambda),
\]

that is,

\[
L(u, \mu) \leq L(u, \lambda) \quad \text{for all } \mu \in \mathbb{R}_+^m \quad (\ast_2)
\]

(since \( \varphi_i(u) \leq 0 \) as \( u \in U \)), and since the function \( v \mapsto J(v) + \sum_{i=1}^m \lambda_i \varphi_i(v) = L(v, \lambda) \) is convex as a sum of convex functions, by Theorem 21.11(4), the first equation is a sufficient condition for the existence of minimum. Consequently,

\[
L(u, \lambda) \leq L(v, \lambda) \quad \text{for all } v \in \Omega, \quad (\ast_3)
\]

and \((\ast_2)\) and \((\ast_3)\) show that \((u, \lambda)\) is a saddle point of \( L \).

To recap what we just proved, under some mild hypotheses, the set of solutions of the minimization Problem \((P)\)

\[
\begin{align*}
\text{minimize} & \quad J(v) \\
\text{subject to} & \quad \varphi_i(v) \leq 0, \quad i = 1, \ldots, m
\end{align*}
\]

coincides with the set of first arguments of the saddle points of the Lagrangian

\[
L(v, \mu) = J(v) + \sum_{i=1}^m \mu_i \varphi_i(v),
\]

and for any optimum \( u \in U \) of Problem \((P)\) we have \( J(u) = L(u, \lambda) \).

Therefore, if we knew some particular second argument \( \lambda \) of these saddle points, then the constrained problem \((P)\) would be replaced by the unconstrained problem \((P_\lambda)\):

\[
\begin{align*}
\text{find } u_\lambda & \in \Omega \text{ such that} \\
L(u_\lambda, \lambda) & = \inf_{v \in \Omega} L(v, \lambda).
\end{align*}
\]

How do we find such an element \( \lambda \in \mathbb{R}_+^m \)?
For this, remember that for a saddle point \((u_\lambda, \lambda)\), by Proposition 31.11, we have

\[
L(u_\lambda, \lambda) = \inf_{v \in \Omega} L(v, \lambda) = \sup_{\mu \in \mathbb{R}_+^m} \inf_{v \in \Omega} L(v, \mu),
\]

so we are naturally led to introduce the function \(G: \mathbb{R}_+^m \to \mathbb{R}\) given by

\[
G(\mu) = \inf_{v \in \Omega} L(v, \mu) \quad \mu \in \mathbb{R}_+^m,
\]

and then \(\lambda\) will be a solution of the problem

\[
\begin{align*}
\text{find } \lambda & \in \mathbb{R}_+^m \text{ such that } \\
G(\lambda) & = \sup_{\mu \in \mathbb{R}_+^m} G(\mu),
\end{align*}
\]

which is equivalent to the maximization problem \((D)\):

\[
\begin{align*}
\text{maximize } & G(\mu) \\
\text{subject to } & \mu \in \mathbb{R}_+^m.
\end{align*}
\]

**Definition 14.9.** Given the minimization problem \((P)\)

\[
\begin{align*}
\text{minimize } & J(v) \\
\text{subject to } & \varphi_i(v) \leq 0, \quad i = 1, \ldots, m,
\end{align*}
\]

where \(J: \Omega \to \mathbb{R}\) and the constraints \(\varphi_i: \Omega \to \mathbb{R}\) are some functions defined on some open subset \(\Omega\) of some finite-dimensional Euclidean vector space \(V\) (more generally, a real Hilbert space \(V\)), the function \(G: \mathbb{R}_+^m \to \mathbb{R}\) given by

\[
G(\mu) = \inf_{v \in \Omega} L(v, \mu) \quad \mu \in \mathbb{R}_+^m,
\]

is called the *Lagrange dual function* (or simply *dual function*). The problem \((D)\)

\[
\begin{align*}
\text{maximize } & G(\mu) \\
\text{subject to } & \mu \in \mathbb{R}_+^m
\end{align*}
\]

is called the *Lagrange dual problem*. The problem \((P)\) is often called the *primal problem*, and \((D)\) is the *dual problem*. The variable \(\mu\) is called the *dual variable*. The variable \(\mu \in \mathbb{R}_+^m\) is said to be *dual feasible* if \(G(\mu)\) is defined (not \(-\infty\)). If \(\lambda \in \mathbb{R}_+^m\) is a maximum of \(G\), then we call it a *dual optimal* or an *optimal Lagrange multiplier*.

Since

\[
L(v, \mu) = J(v) + \sum_{i=1}^m \mu_i \varphi_i(v),
\]
the function \( G(\mu) = \inf_{v \in \Omega} L(v, \mu) \) is the pointwise infimum of some affine functions of \( \mu \), so it is concave, even if the \( \varphi_i \) are not convex. One of the main advantages of the dual problem over the primal problem is that it is a convex optimization problem, since we wish to maximize a concave objective function \( G \) (thus minimize \(-G\), a convex function), and the constraints \( \mu \geq 0 \) are convex. In a number of practical situations the dual function \( G \) can indeed be computed.

To be perfectly rigorous we should mention that the dual function \( G \) is actually a partial function, because it takes the value \(-\infty\) when the map \( v \mapsto L(v, \mu) \) is unbounded below.

**Example 14.5.** Consider the linear program \((P)\)

\[
\begin{align*}
\text{minimize} & \quad c^\top v \\
\text{subject to} & \quad Av \leq b, \ v \geq 0,
\end{align*}
\]

where \( A \) is an \( m \times n \) matrix. The constraints \( v \geq 0 \) are rewritten as \(-v_i \leq 0\), so we introduce Lagrange multipliers \( \mu \in \mathbb{R}^m_+ \) and \( \nu \in \mathbb{R}^n_+ \), and we have the Lagrangian

\[
L(v, \mu, \nu) = c^\top v + \mu^\top (Av - b) - \nu^\top v \\
= -b^\top \mu + (c + A^\top \mu - \nu)^\top v.
\]

The linear function \( v \mapsto (c + A^\top \mu - \nu)^\top v \) is unbounded below unless \( c + A^\top \mu - \nu = 0 \), so the dual function \( G(\mu, \nu) = \inf_{v \in \mathbb{R}^n} L(v, \mu, \nu) \) is given for all \( \mu \geq 0 \) and \( \nu \geq 0 \) by

\[
G(\mu, \nu) = \begin{cases} 
- b^\top \mu & \text{if } A^\top \mu - \nu + c = 0, \\
-\infty & \text{otherwise}.
\end{cases}
\]

The domain of \( G \) is a proper subset of \( \mathbb{R}^m_+ \times \mathbb{R}^n_+ \).

Observe that the value \( G(\mu, \nu) \) of the function \( G \), when it is defined, is independent of the second argument \( \nu \). Since we are interested in maximizing \( G \), this suggests introducing the function \( \hat{G} \) of the single argument \( \mu \) given by

\[
\hat{G}(\mu) = -b^\top \mu,
\]

which is defined for all \( \mu \in \mathbb{R}^m_+ \).

Of course, \( \sup_{\mu \in \mathbb{R}^m_+} \hat{G}(\mu) \) and \( \sup_{(\mu, \nu) \in \mathbb{R}^m_+ \times \mathbb{R}^n_+} G(\mu, \nu) \) are generally different, but note that \( \hat{G}(\mu) = G(\mu, \nu) \) iff there is some \( \nu \in \mathbb{R}^n_+ \) such that \( A^\top \mu - \nu + c = 0 \) iff \( A^\top \mu + c \geq 0 \). Therefore, finding \( \sup_{(\mu, \nu) \in \mathbb{R}^m_+ \times \mathbb{R}^n_+} G(\mu, \nu) \) is equivalent to the constrained problem \((D_1)\)

\[
\begin{align*}
\text{maximize} & \quad - b^\top \mu \\
\text{subject to} & \quad A^\top \mu \geq -c, \ \mu \geq 0.
\end{align*}
\]

The above problem is the dual of the linear program \((P)\).
In summary, the dual function $G$ of a primary problem $(P)$ often contains hidden inequality constraints that define its domain, and sometimes it is possible to make these domain constraints $\psi_1(\mu) \leq 0, \ldots, \psi_p(\mu) \leq 0$ explicit, to define a new function $\hat{G}$ that depends only on $q < m$ of the variables $\mu_i$ and is defined for all values $\mu_i \geq 0$ of these variables, and to replace the maximization problem $(D)$, find $\sup_{\mu \in \mathbb{R}^m_+} G(\mu)$, by the constrained problem $(D_1)$

\[
\begin{align*}
\text{maximize} & \quad \hat{G}(\mu) \\
\text{subject to} & \quad \psi_i(\mu) \leq 0, \quad i = 1, \ldots, p.
\end{align*}
\]

Problem $(D_1)$ is different from the dual program $(D)$, but it is equivalent to $(D)$ as a maximization problem.

Another important property of the dual function $G$ is that it provides a lower bound on the value of the objective function $J$. Indeed, we have

\[
G(\mu) \leq L(u, \mu) \leq J(u) \quad \text{for all } u \in U \text{ and all } \mu \in \mathbb{R}^m_+, \tag{\dagger}
\]

since $\mu \geq 0$ and $\varphi_i(u) \leq 0$ for $i = 1, \ldots, m$, so

\[
G(\mu) = \inf_{v \in \Omega} L(v, \mu) \leq L(u, \mu) = J(u) + \sum_{i=1}^{m} \mu_i \varphi_i(u) \leq J(u).
\]

If the primal problem $(P)$ has a minimum denoted $p^*$ and the dual problem $(D)$ has a maximum denoted $d^*$, then the above inequality implies that

\[
d^* \leq p^*, \tag{\dagger_w}
\]

known as weak duality. Equivalently, for every optimal solution $\lambda^*$ of the dual problem and every optimal solution $u^*$ of the primal problem, we have

\[
G(\lambda^*) \leq J(u^*). \tag{\dagger_{w'}}
\]

In particular, if $p^* = -\infty$, which means that the primal problem is unbounded below, then the dual problem is unfeasible. Conversely, if $d^* = +\infty$, which means that the dual problem is unbounded above, then the primal problem is unfeasible.

The difference $p^* - d^* \geq 0$ is called the optimal duality gap. If the duality gap is zero, that is, $p^* = d^*$, then we say that strong duality holds. Even when the duality gap is strictly positive, the inequality $(\dagger_w)$ can be helpful to find a lower bound on the optimal value of a primal problem that is difficult to solve, since the dual problem is always convex.

If the primal problem and the dual problem are feasible and if the optimal values $p^*$ and $d^*$ are finite and $p^* = d^*$ (no duality gap), then the complementary slackness conditions hold for the inequality constraints.
Proposition 14.13. (Complementary Slackness) Given the minimization problem \((P)\)

\[
\begin{align*}
\text{minimize} & \quad J(v) \\
\text{subject to} & \quad \varphi_i(v) \leq 0, \quad i = 1, \ldots, m,
\end{align*}
\]

and its dual problem \((D)\)

\[
\begin{align*}
\text{maximize} & \quad G(\mu) \\
\text{subject to} & \quad \mu \in \mathbb{R}_+^m,
\end{align*}
\]

if both \((P)\) and \((D)\) are feasible, \(u \in U\) is an optimal solution of \((P)\), \(\lambda \in \mathbb{R}_+^m\) is an optimal solution of \((D)\), and \(J(u) = G(\lambda)\), then

\[
\sum_{i=1}^{m} \lambda_i \varphi_i(u) = 0.
\]

In other words, if the constraint \(\varphi_i\) is inactive at \(u\), then \(\lambda_i = 0\).

Proof. Since \(J(u) = G(\lambda)\) we have

\[
\begin{align*}
J(u) &= G(\lambda) \\
&= \inf_{v \in \Omega} \left( J(v) + \sum_{i=1}^{m} \lambda_i \varphi_i(v) \right) \quad \text{by definition of } G \\
&\leq J(u) + \sum_{i=1}^{m} \lambda_i \varphi_i(u) \quad \text{the greatest lower bound is a lower bound} \\
&\leq J(u) \quad \text{since } \lambda_i \geq 0, \varphi_i(u) \leq 0.
\end{align*}
\]

which implies that \(\sum_{i=1}^{m} \lambda_i \varphi_i(u) = 0\). \(\square\)

Going back to Example 31.5, we see that weak duality says that for any feasible solution \(u\) of the primal problem \((P)\), that is, some \(u \in \mathbb{R}^n\) such that

\[
Au \leq b, \quad u \geq 0,
\]

and for any feasible solution \(\mu \in \mathbb{R}^m\) of the dual problem \((D)\), that is,

\[
A^\top \mu \geq -c, \quad \mu \geq 0,
\]

we have

\[
-b^\top \mu \leq c^\top u.
\]

Actually, if \(u\) and \(\lambda\) are optimal, then we know that strong duality holds, namely \(-b^\top \mu = c^\top u\), but the proof of this fact is nontrivial.

The following theorem establishes a link between the solutions of the primal problem \((P)\) and those of the dual problem \((D)\). It also gives sufficient conditions for the duality gap to be zero.
\[
\begin{align*}
\text{minimize} & \quad J(v) \\
\text{subject to} & \quad \varphi_i(v) \leq 0, \quad i = 1, \ldots, m,
\end{align*}
\]
where the functions \(J\) and \(\varphi_i\) are defined on some open subset \(\Omega\) of a finite-dimensional Euclidean vector space \(V\) (more generally, a real Hilbert space \(V\)).

(1) Suppose the functions \(\varphi_i : \Omega \rightarrow \mathbb{R}\) are continuous, and that for every \(\mu \in \mathbb{R}^m_+\), the problem \((P_\mu)\):
\[
\begin{align*}
\text{minimize} & \quad L(v, \mu) \\
\text{subject to} & \quad v \in \Omega,
\end{align*}
\]
has a unique solution \(u_\mu\), so that
\[
L(u_\mu, \mu) = \inf_{v \in \Omega} L(v, \mu) = G(\mu),
\]
and the function \(\mu \mapsto u_\mu\) is continuous (on \(\mathbb{R}^m_+\)). If \(\lambda\) is any solution of problem \((D)\):
\[
\begin{align*}
\text{maximize} & \quad G(\mu) \\
\text{subject to} & \quad \mu \in \mathbb{R}^m_+,
\end{align*}
\]
then the solution \(u_\lambda\) of the corresponding problem \((P_\lambda)\) is a solution of Problem \((P)\).

(2) Assume Problem \((P)\) has some solution \(u \in U\), and that \(\Omega\) is convex (open), the functions \(\varphi_i\) \((1 \leq i \leq m)\) and \(J\) are convex and differentiable at \(u\), and that the constraints are qualified. Then Problem \((D)\) has a solution \(\lambda \in \mathbb{R}^m_+\), and \(J(u) = G(\lambda)\); that is, the duality gap is zero.

Proof. (1) Our goal is to prove that for any solution \(\lambda\) of Problem \((D)\), the pair \((u_\lambda, \lambda)\) is a saddle point of \(L\). By Theorem 31.12(1), the point \(u_\lambda \in U\) is a solution of Problem \((P)\).

Since \(\lambda \in \mathbb{R}^m_+\) is a solution of Problem \((D)\), by definition of \(G(\lambda)\) and since \(u_\lambda\) satisfies Problem \((P_\lambda)\), we have
\[
G(\lambda) = \inf_{v \in \Omega} L(v, \lambda) = L(u_\lambda, \lambda),
\]
which is one of the two equations characterizing a saddle point. In order to prove the second equation characterizing a saddle point,
\[
\sup_{\mu \in \mathbb{R}^m_+} L(u_\mu, \mu) = L(u_\lambda, \lambda),
\]
we will begin by proving that the function \(G\) is differentiable for any \(\mu \in \mathbb{R}^m_+\), in order to be able to apply Theorem 21.8 to conclude that since \(G\) has a maximum at \(\lambda\), that is, \(-G\) has minimum at \(\lambda\), then \(-G'_\lambda(\mu - \lambda) \geq 0\) for all \(\mu \in \mathbb{R}^m_+\). In fact, we prove that
\[
G'_\mu(\xi) = \sum_{i=1}^m \xi_i \varphi_i(u_\mu) \quad \text{for all} \ \xi \in \mathbb{R}^m.
\]
Consider any two points $\mu$ and $\mu + \xi$ in $\mathbb{R}^m$. By definition of $u_\mu$ we have

$$L(u_\mu, \mu) \leq L(u_{\mu+\xi}, \mu),$$

which means that

$$J(u_\mu) + \sum_{i=1}^{m} \mu_i \varphi_i(u_\mu) \leq J(u_{\mu+\xi}) + \sum_{i=1}^{m} \mu_i \varphi_i(u_{\mu+\xi}), \quad (*)_1$$

and since $G(\mu) = L(u_\mu, \mu) = J(u_\mu) + \sum_{i=1}^{m} \mu_i \varphi_i(u_\mu)$ and $G(\mu + \xi) = L(u_{\mu+\xi}, \mu + \xi) = J(u_{\mu+\xi}) + \sum_{i=1}^{m} (\mu_i + \xi_i) \varphi_i(u_{\mu+\xi})$, we have

$$G(\mu + \xi) - G(\mu) = J(u_{\mu+\xi}) - J(u_\mu) + \sum_{i=1}^{m} (\mu_i + \xi_i) \varphi_i(u_{\mu+\xi}) - \sum_{i=1}^{m} \mu_i \varphi_i(u_\mu), \quad (*)_2$$

and since $(*)_1$ can be written as

$$0 \leq J(u_{\mu+\xi}) - J(u_\mu) + \sum_{i=1}^{m} \mu_i \varphi_i(u_{\mu+\xi}) - \sum_{i=1}^{m} \mu_i \varphi_i(u_\mu),$$

by adding $\sum_{i=1}^{m} \xi_i \varphi_i(u_{\mu+\xi})$ to both sides of the above inequality and using $(*)_2$ we get

$$\sum_{i=1}^{m} \xi_i \varphi_i(u_{\mu+\xi}) \leq G(\mu + \xi) - G(\mu). \quad (**)_3$$

By definition of $u_{\mu+\xi}$ we have

$$L(u_{\mu+\xi}, \mu + \xi) \leq L(u_\mu, \mu + \xi),$$

which means that

$$J(u_{\mu+\xi}) + \sum_{i=1}^{m} (\mu_i + \xi_i) \varphi_i(u_{\mu+\xi}) \leq J(u_\mu) + \sum_{i=1}^{m} (\mu_i + \xi_i) \varphi_i(u_\mu), \quad (**)_4$$

which can be written as

$$J(u_{\mu+\xi}) - J(u_\mu) + \sum_{i=1}^{m} (\mu_i + \xi_i) \varphi_i(u_{\mu+\xi}) - \sum_{i=1}^{m} (\mu_i + \xi_i) \varphi_i(u_\mu) \leq 0,$$

and by adding $\sum_{i=1}^{m} \xi_i \varphi_i(u_\mu)$ to both sides of the above inequality and using $(*)_2$ we get

$$G(\mu + \xi) - G(\mu) \leq \sum_{i=1}^{m} \xi_i \varphi_i(u_\mu). \quad (**)_5$$
Putting \((\ast_3)\) and \((\ast_5)\) together we obtain
\[
\sum_{i=1}^{m} \xi_i \varphi_i(u_{\mu+\xi}) \leq G(\mu + \xi) - G(\mu) \leq \sum_{i=1}^{m} \xi_i \varphi_i(u_{\mu}).
\] \((\ast_6)\)

Consequently there is some \(\theta \in [0, 1]\) such that
\[
G(\mu + \xi) - G(\mu) = (1 - \theta) \left( \sum_{i=1}^{m} \xi_i \varphi_i(u_{\mu}) \right) + \theta \left( \sum_{i=1}^{m} \xi_i \varphi_i(u_{\mu+\xi}) \right)
\]
\[
= \sum_{i=1}^{m} \xi_i \varphi_i(u_{\mu}) + \theta \left( \sum_{i=1}^{m} \xi_i (\varphi_i(u_{\mu+\xi}) - \varphi_i(u_{\mu})) \right).
\]

Since by hypothesis the functions \(\mu \mapsto u_{\mu}\) (from \(\mathbb{R}^m_+\) to \(\Omega\)) and \(\varphi_i: \Omega \to \mathbb{R}\) are continuous, for any \(\mu \in \mathbb{R}^m_+\) we can write
\[
G(\mu + \xi) - G(\mu) = \sum_{i=1}^{m} \xi_i \varphi_i(u_{\mu}) + \|\xi\| \epsilon(\xi), \quad \text{with } \lim_{\xi \to 0} \epsilon(\xi) = 0,
\]
\((\ast_7)\)

for any \(\|\|\) norm on \(\mathbb{R}^m\). Equation \((\ast_7)\) show that \(G\) is differentiable for any \(\mu \in \mathbb{R}^m_+\), and that
\[
G'_\mu(\xi) = \sum_{i=1}^{m} \xi_i \varphi_i(u_{\mu}) \quad \text{for all } \xi \in \mathbb{R}^m.
\]
\((\ast_8)\)

Actually there is a small problem, namely that the notion of derivative was defined for a function defined on an open set, but \(\mathbb{R}^m_+\) is not open. The difficulty only arises to ensure that the derivative is unique, but in our case we have a unique expression for the derivative so there is no problem as far as defining the derivative. There is still a potential problem, which is that we would like to apply Theorem 21.8 to conclude that since \(G\) has a maximum at \(\lambda\), that is, \(-G\) has minimum at \(\lambda\), then
\[
-G'_\lambda(\mu - \lambda) \geq 0 \quad \text{for all } \mu \in \mathbb{R}^m_+,
\]
\((\ast_9)\)

but the hypotheses of Theorem 21.8 require the domain of the function to be open. Fortunately, close examination of the proof of Theorem 21.8 shows that the proof still holds with \(U = \mathbb{R}^m_+\). Therefore, \((\ast_8)\) holds, equivalently
\[
G'_\lambda(\mu - \lambda) \leq 0 \quad \text{for all } \mu \in \mathbb{R}^m_+,
\]
\((\ast_{10})\)

which, using the expression for \(G'_\lambda\) given in \((\ast_8)\) gives
\[
\sum_{i=1}^{m} \mu_i \varphi_i(u_{\lambda}) \leq \sum_{i=1}^{m} \lambda_i \varphi_i(u_{\lambda}), \quad \text{for all } \mu \in \mathbb{R}^m_+.
\]
\((\ast_{11})\)
As a consequence of (\(\ast_{11}\)), we obtain
\[
L(u_\lambda, \mu) = J(u_\lambda) + \sum_{i=1}^{m} \mu_i \varphi_i(u_\lambda)
\leq J(u_\lambda) + \sum_{i=1}^{m} \lambda_i \varphi_i(u_\lambda) = L(u_\lambda, \lambda),
\]
for all \(\mu \in \mathbb{R}_+^m\), that is,
\[
L(u_\lambda, \mu) \leq L(u_\lambda, \lambda), \quad \text{for all } \mu \in \mathbb{R}_+^m, \tag{\(\ast_{12}\)}
\]
which implies the second inequality
\[
\sup_{\mu \in \mathbb{R}_+^m} L(u_\mu, \mu) = L(u_\lambda, \lambda)
\]
stating that \((u_\lambda, \lambda)\) is a saddle point. Therefore, \((u_\lambda, \lambda)\) is a saddle point of \(L\), as claimed.

(2) The hypotheses are exactly those required by Theorem 31.12(2), thus there is some \(\lambda \in \mathbb{R}_+^m\) such that \((u, \lambda)\) is a saddle point of the Lagrangian \(L\), and by Theorem 31.12(1) we have \(J(u) = L(u, \lambda)\). By Proposition 31.11, we have
\[
J(u) = L(u, \lambda) = \inf_{v \in \Omega} L(v, \lambda) = \sup_{\mu \in \mathbb{R}_+^m} \inf_{v \in \Omega} L(v, \mu),
\]
which can be rewritten as
\[
J(u) = G(\lambda) = \sup_{\mu \in \mathbb{R}_+^m} G(\mu),
\]
in other words, Problem \((D)\) has a solution, and \(J(u) = G(\lambda)\). \hfill \square

Remark: If \((u, \lambda)\) is a saddle point of the Lagrangian \(L\) (defined on \(\Omega \times \mathbb{R}_+^m\)), then by Proposition 31.11 the vector \(\lambda\) is a solution of Problem \((D)\). Conversely, under the hypotheses of Part (1) of Theorem 31.14, if \(\lambda\) is a solution of Problem \((D)\), then \((u_\lambda, \lambda)\) is a saddle point of \(L\). Consequently, under the above hypotheses, the set of solutions of the dual problem \((D)\) coincide with the set of second arguments \(\lambda\) of the saddle points \((u, \lambda)\) of \(L\). In some sense, this result is the “dual” of the result stated in Theorem 31.12, namely that the set of solutions of Problem \((P)\) coincides with set of first arguments \(u\) of the saddle points \((u, \lambda)\) of \(L\).

Informally, in Theorem 31.14(1), the hypotheses say that if \(G(\mu)\) can be “computed nicely,” in the sense that there is a unique minimizer \(u_\mu\) of \(L(v, \mu)\) (with \(v \in \Omega\)) such that \(G(\mu) = L(u_\mu, \mu)\), and if a maximizer \(\lambda\) of \(G(\mu)\) (with \(\mu \in \mathbb{R}_+^m\)) can be determined, then \(u_\lambda\) yields the minimum value of \(J\), that is, \(p^* = J(u_\lambda)\). If the constraints are qualified and if the functions \(J\) and \(\varphi_i\) are convex and differentiable, then since the KKT conditions hold, the duality gap is zero; that is,
\[
G(\lambda) = L(u_\lambda, \lambda) = J(u_\lambda).
\]
Example 14.6. Going back to Example 31.5 where we considered the linear program \((P)\)

\[
\begin{align*}
\text{minimize} & \quad c^\top v \\
\text{subject to} & \quad Av \leq b, \; v \geq 0,
\end{align*}
\]

with \(A\) an \(m \times n\) matrix, the Lagrangian \(L(\mu, \nu)\) is given by

\[
L(v, \mu, \nu) = -b^\top \mu + (c + A^\top \mu - \nu)^\top v,
\]

and we found that the dual function \(G(\mu, \nu) = \inf_{v \in \mathbb{R}^n} L(v, \mu, \nu)\) is given for all \(\mu \geq 0\) and \(\nu \geq 0\) by

\[
G(\mu, \nu) = \begin{cases}
-b^\top \mu & \text{if } A^\top \mu - \nu + c = 0, \\
-\infty & \text{otherwise}.
\end{cases}
\]

The hypotheses of Theorem 31.14(1) certainly fail since there are infinitely \(u_{\mu, \nu} \in \mathbb{R}^n\) such that \(G(\mu, \nu) = \inf_{v \in \mathbb{R}^n} L(v, \mu, \nu) = L(u_{\mu, \nu}, \mu, \nu)\). Therefore, the dual function \(G\) is no help in finding a solution of the primal \((P)\). As we saw earlier, if we consider the modified dual Problem \((D_1)\) then strong duality holds, but this does not follow from Theorem 31.14, and a different proof is required.

Thus we have the somewhat counter-intuitive situation that the general theory of Lagrange duality does not apply, at least directly, to linear programming, a fact that is not sufficiently emphasized in many expositions. A separate treatment of duality if required.

Unlike the case of linear programming, which needs a separate treatment, Theorem 31.14 applies to the optimization problem involving a convex quadratic objective function and a set of affine inequality constraints. So in some sense, convex quadratic programming is simpler than linear programming!

Example 14.7. Consider the quadratic objective function

\[
J(v) = \frac{1}{2} v^\top A v - v^\top b,
\]

where \(A\) is an \(n \times n\) matrix which is symmetric positive definite, \(b \in \mathbb{R}^n\), and the constraints are affine inequality constraints of the form

\[
C v \leq d,
\]

where \(C\) is an \(m \times n\) matrix and \(d \in \mathbb{R}^m\). For the time being, we do not assume that \(C\) has rank \(m\). Since \(A\) is symmetric positive definite, \(J\) is strictly convex, as implied by Proposition 21.9 (see Example 21.1). The Lagrangian of this quadratic optimization problem is given by

\[
L(v, \mu) = \frac{1}{2} v^\top A v - v^\top b + (C v - d)^\top \mu \\
= \frac{1}{2} v^\top A v - v^\top (b - C^\top \mu) - \mu^\top d.
\]
Since \( A \) is symmetric positive definite, by Proposition 23.2, the function \( v \mapsto L(v, \mu) \) has a unique minimum obtained for the solution \( u_\mu \) of the linear system

\[
Av = b - C^\top \mu;
\]

that is,

\[
u_\mu = A^{-1}(b - C^\top \mu).
\]

This shows that the Problem \((P_\mu)\) has a unique solution which depends continuously on \( \mu \). Then for any solution \( \lambda \) of the dual problem, \( u_\lambda = A^{-1}(b - C^\top \lambda) \) is an optimal solution of the primal problem.

We compute \( G(\mu) \) as follows:

\[
G(\mu) = L(u_\mu, \mu) = \frac{1}{2} u_\mu^\top Au_\mu - u_\mu^\top (b - C^\top \mu) - \mu^\top d
\]

\[
= \frac{1}{2} u_\mu^\top (b - C^\top \mu) - u_\mu^\top (b - C^\top \mu) - \mu^\top d
\]

\[
= -\frac{1}{2} u_\mu^\top (b - C^\top \mu) - \mu^\top d
\]

\[
= -\frac{1}{2} (b - C^\top \mu)^\top A^{-1}(b - C^\top \mu) - \mu^\top d
\]

\[
= -\frac{1}{2} \mu^\top CA^{-1}C^\top \mu + \mu^\top (CA^{-1}b - d) - \frac{1}{2} b^\top A^{-1}b.
\]

Since \( A \) is symmetric positive definite, the matrix \( CA^{-1}C^\top \) is symmetric positive semidefinite. Since \( A^{-1} \) is also symmetric positive definite, \( \mu^\top CA^{-1}C^\top \mu = 0 \) iff \( (C^\top \mu)^\top A^{-1}(C^\top \mu) = 0 \) iff \( C^\top \mu = 0 \) implies \( \mu = 0 \), that is, \( \text{Ker} C^\top = (0) \), which is equivalent to \( \text{Im}(C) = \mathbb{R}^m \), namely if \( C \) has rank \( m \) (in which case, \( m \leq n \)). Thus \( CA^{-1}C^\top \) is symmetric positive definite iff \( C \) has rank \( m \).

We showed just after Theorem 30.7 that the functional \( v \mapsto (1/2)v^\top Av \) is elliptic iff \( A \) is symmetric positive definite, and Theorem 30.7 shows that an elliptic functional is coercive, which is the hypothesis used in Theorem 30.3. Therefore, by Theorem 30.3, if the inequalities \( Cx \leq d \) have a solution, the primal problem has a unique solution. In this case, as a consequence, by Theorem 31.14(2), the function \( -G(\mu) \) always has a minimum, which is unique if \( C \) has rank \( m \). The fact that \( -G(\mu) \) has a minimum is not obvious when \( C \) has rank \( < m \), since in this case \( CA^{-1}C^\top \) is not invertible.

We also verify easily that the gradient of \( G \) is given by

\[
\nabla G_\mu = Cu_\mu - d = -CA^{-1}C^\top \mu + CA^{-1}b - d.
\]

Observe that since \( CA^{-1}C^\top \) is symmetric positive semidefinite, \( -G(\mu) \) is convex.

Therefore, if \( C \) has rank \( m \), a solution of Problem \((P)\) is obtained by finding the unique solution \( \lambda \) of the equation

\[
-CA^{-1}C^\top \mu + CA^{-1}b - d = 0,
\]
and then the minimum $u_\lambda$ of Problem \((P)\) is given by

$$u_\lambda = A^{-1}(b - C^T \lambda).$$

If \(C\) has rank \(< m\), then we can find \(\lambda \geq 0\) by finding a feasible solution of the linear program whose set of constraints is given by

$$-CA^{-1}C^T \mu + CA^{-1}b - d = 0,$$

using the standard method of adding nonnegative slack variables $\xi_1, \ldots, \xi_m$ and maximizing $-(\xi_1 + \cdots + \xi_m)$.

### 14.6 Handling Equality Constraints Explicitly

Sometimes it is desirable to handle equality constraints explicitly (for instance, this is what Boyd and Vandenberghe do, see [22]). The only difference is that the Lagrange multipliers associated with equality constraints are not required to be nonnegative, as we now show.

Consider the optimization problem \((P')\)

$$\begin{align*}
\text{minimize} & \quad J(v) \\
\text{subject to} & \quad \varphi_i(v) \leq 0, \quad i = 1, \ldots, m \\
& \quad \psi_j(v) = 0, \quad j = 1, \ldots, p.
\end{align*}$$

We treat each equality constraint $\psi_j(u) = 0$ as the conjunction of the inequalities $\psi_j(u) \leq 0$ and $-\psi_j(u) \leq 0$, and we associate Lagrange multipliers $\lambda \in \mathbb{R}^m_+$, and $\nu^+, \nu^- \in \mathbb{R}^p_+$. The KKT conditions are

$$\begin{align*}
J'_u + \sum_{i=1}^m \lambda_i \varphi_i'(u) + \sum_{j=1}^p \nu_j^+(\psi_j' u) - \sum_{j=1}^p \nu_j^-(\psi_j' u) &= 0, \\
\sum_{i=1}^m \lambda_i \varphi_i(u) + \sum_{j=1}^p \nu_j^+ \psi_j(u) - \sum_{j=1}^p \nu_j^- \psi_j(u) &= 0,
\end{align*}$$

with $\lambda \geq 0, \nu^+ \geq 0, \nu^- \geq 0$. Since $\psi_j(u) = 0$ for $j = 1, \ldots, p$, these equations can be rewritten as

$$\begin{align*}
J'_u + \sum_{i=1}^m \lambda_i \varphi_i'(u) + \sum_{j=1}^p (\nu_j^+ - \nu_j^-)(\psi_j' u) &= 0, \\
\sum_{i=1}^m \lambda_i \varphi_i(u) &= 0
\end{align*}$$
with $\lambda \geq 0$, $\nu^+ \geq 0$, $\nu^- \geq 0$, and if we introduce $\nu_j = \nu^+_j - \nu^-_j$ we obtain the following KKT conditions for programs with explicit equality constraints:

$$J'_u + \sum_{i=1}^{m} \lambda_i (\varphi'_i)u + \sum_{j=1}^{p} \nu_j (\psi'_j)u = 0,$$

and

$$\sum_{i=1}^{m} \lambda_i \varphi_i(u) = 0$$

with $\lambda \geq 0$ and $\nu \in \mathbb{R}^p$ arbitrary.

Let us now assume that the functions $\varphi_i$ and $\psi_j$ are convex. As we explained just after Definition 31.6, nonaffine equality constraints are never qualified. Thus, in order to generalize Theorem 31.6 to explicit equality constraints, we assume that the equality constraints $\psi_j$ are affine.

**Theorem 14.15.** Let $\varphi_i: \Omega \to \mathbb{R}$ be $m$ convex inequality constraints and $\psi_j: \Omega \to \mathbb{R}$ be $p$ affine equality constraints defined on some open convex subset $\Omega$ of a finite-dimensional Euclidean vector space $V$ (more generally, a real Hilbert space $V$), let $J: \Omega \to \mathbb{R}$ be some function, let $U$ be given by

$$U = \{x \in \Omega \mid \varphi_i(x) \leq 0, \; \psi_j(x) = 0, \; 1 \leq i \leq m, \; 1 \leq j \leq p\};$$

and let $u \in U$ be any point such that the functions $\varphi_i$ and $J$ are differentiable at $u$, and the functions $\psi_j$ are affine.

(1) If $J$ has a local minimum at $u$ with respect to $U$, and if the constraints are qualified, then there exist some vectors $\lambda \in \mathbb{R}^m_+$ and $\nu \in \mathbb{R}^p$, such that the KKT condition hold:

$$J'_u + \sum_{i=1}^{m} \lambda_i (\varphi'_i)u + \sum_{j=1}^{p} \nu_j (\psi'_j)u = 0,$$

and

$$\sum_{i=1}^{m} \lambda_i \varphi_i(u) = 0, \quad \lambda_i \geq 0, \quad i = 1, \ldots, m.$$

Equivalently, in terms of gradients, the above conditions are expressed as

$$\nabla J_u + \sum_{i=1}^{m} \lambda_i \nabla (\varphi_i)u + \sum_{j=1}^{p} \nu_j \nabla (\psi_j)u = 0$$

and

$$\sum_{i=1}^{m} \lambda_i \varphi_i(u) = 0, \quad \lambda_i \geq 0, \quad i = 1, \ldots, m.$$
(2) Conversely, if the restriction of $J$ to $U$ is convex and if there exist vectors $\lambda \in \mathbb{R}^m_+$ and $\nu \in \mathbb{R}^p$ such that the KKT conditions hold, then the function $J$ has a (global) minimum at $u$ with respect to $U$.

The Lagrangian $L(v, \lambda, \nu)$ of Problem $(P')$ is defined as

$$L(v, \mu, \nu) = J(v) + \sum_{i=1}^{m} \mu_i \varphi_i(v) + \sum_{j=1}^{p} \nu_j \psi_j(v),$$

where $v \in \Omega$, $\mu \in \mathbb{R}^m_+$, and $\nu \in \mathbb{R}^p$.

The function $G: \mathbb{R}^m_+ \times \mathbb{R}^p \to \mathbb{R}$ given by

$$G(\mu, \nu) = \inf_{v \in \Omega} L(v, \mu, \nu) \quad \mu \in \mathbb{R}^m_+, \nu \in \mathbb{R}^p$$

is called the Lagrange dual function (or dual function), and the dual problem $(D')$ is

$$\begin{align*}
\text{maximize} & \quad G(\mu, \nu) \\
\text{subject to} & \quad \mu \in \mathbb{R}^m_+, \nu \in \mathbb{R}^p.
\end{align*}$$

Observe that the Lagrange multipliers $\nu$ are not restricted to be nonnegative.

Theorem 31.12 and Theorem 31.14 are immediately generalized to Problem $(P')$. We only state the new version of 31.14, leaving the new version of Theorem 31.12 as an exercise.

**Theorem 14.16.** Consider the minimization problem $(P')$:

$$\begin{align*}
\text{minimize} & \quad J(v) \\
\text{subject to} & \quad \varphi_i(v) \leq 0, \quad i = 1, \ldots, m \\
& \quad \psi_j(v) = 0, \quad j = 1, \ldots, p.
\end{align*}$$

where the functions $J, \varphi_i$ are defined on some open subset $\Omega$ of a finite-dimensional Euclidean vector space $V$ (more generally, a real Hilbert space $V$), and the functions $\psi_j$ are affine.

(1) Suppose the functions $\varphi_i: \Omega \to \mathbb{R}$ are continuous, and that for every $\mu \in \mathbb{R}^m_+$ and every $\nu \in \mathbb{R}^p$, the problem $(P_{\mu,\nu})$:

$$\begin{align*}
\text{minimize} & \quad L(v, \mu, \nu) \\
\text{subject to} & \quad v \in \Omega,
\end{align*}$$

has a unique solution $u_{\mu,\nu}$, so that

$$L(u_{\mu,\nu}, \mu, \nu) = \inf_{v \in \Omega} L(v, \mu, \nu) = G(\mu, \nu),$$

and the function $(\mu, \nu) \mapsto u_{\mu,\nu}$ is continuous (on $\mathbb{R}^m_+ \times \mathbb{R}^p$). If $(\lambda, \eta)$ is any solution of problem $(D)$:

$$\begin{align*}
\text{maximize} & \quad G(\mu, \nu) \\
\text{subject to} & \quad \mu \in \mathbb{R}^m_+, \nu \in \mathbb{R}^p,
\end{align*}$$

then the solution $u_{\lambda,\eta}$ of the corresponding problem $(P_{\lambda,\eta})$ is a solution of Problem $(P')$. 

Assume Problem \((P')\) has some solution \(u \in U\), and that \(\Omega\) is convex (open), the functions \(\varphi_i\) \((1 \leq i \leq m)\) and \(J\) are convex, differentiable at \(u\), and that the constraints are qualified. Then Problem \((D')\) has a solution \((\lambda, \eta) \in \mathbb{R}^m_+ \times \mathbb{R}^p\), and \(J(u) = G(\lambda, \eta)\); that is, the duality gap is zero.

In the next example we derive the dual function and the dual program of the optimization problem of Section 31.4 (Hard margin SVM), which involves both inequality and equality constraints. We also derive the KKT conditions associated with the dual program.

**Example 14.8.** Recall the Hard margin SVM problem (SVM\(_{h2}\)):

\[
\begin{align*}
\text{minimize} \quad & \frac{1}{2} \|w\|^2 \\
\text{subject to} \quad & w^\top u_i - b \geq 1 \quad i = 1, \ldots, p \\
& -w^\top v_j + b \geq 1 \quad j = 1, \ldots, q.
\end{align*}
\]

We proceed in six steps.

**Step 1:** Write the constraints in matrix form.

The inequality constraints are written as

\[
C \begin{pmatrix} w \\ b \end{pmatrix} \leq d,
\]

where \(C\) is a \((p + q) \times (n + 1)\) matrix \(C\) and \(d \in \mathbb{R}^{p+q}\) is the vector given by

\[
C = \begin{pmatrix}
-u_1^\top & 1 \\
\vdots & \vdots \\
-u_p^\top & 1 \\
v_1^\top & -1 \\
\vdots & \vdots \\
v_q^\top & -1
\end{pmatrix}, \quad d = \begin{pmatrix} -1 \\ \vdots \\ -1 \end{pmatrix} = -1_{p+q}.
\]

If let \(X\) be the \(n \times (p + q)\) matrix given by

\[
X = \begin{pmatrix} -u_1 & \cdots & -u_p & v_1 & \cdots & v_q \end{pmatrix},
\]

then

\[
C = \begin{pmatrix} X^\top 1_p \\ -1_q \end{pmatrix}
\]

and so

\[
C^\top = \begin{pmatrix} 1_p^\top & X \\ 1_q & -1_q^\top \end{pmatrix}.
\]
**Step 2:** Write the objective function in matrix form.

The objective function is given by

$$J(w, b) = \frac{1}{2} \begin{pmatrix} w^\top & b \end{pmatrix} \begin{pmatrix} I_n & 0_n \\ 0_n & 0 \end{pmatrix} \begin{pmatrix} w \\ b \end{pmatrix}.$$ 

Note that the corresponding matrix is symmetric positive semidefinite, but it is not invertible. Thus the function $J$ is convex but not strictly convex.

**Step 3:** Write the Lagrangian in matrix form.

As in Example 31.7, we obtain the Lagrangian

$$L(w, b, \lambda, \mu) = \frac{1}{2} \begin{pmatrix} w^\top & b \end{pmatrix} \begin{pmatrix} I_n & 0_n \\ 0_n & 0 \end{pmatrix} \begin{pmatrix} w \\ b \end{pmatrix} - \begin{pmatrix} w^\top & b \end{pmatrix} \begin{pmatrix} 0_{n+1} - C^\top \begin{pmatrix} \lambda \\ \mu \end{pmatrix} \end{pmatrix} + \begin{pmatrix} \lambda^\top & \mu^\top \end{pmatrix} \begin{pmatrix} 1_p + 1_q \end{pmatrix},$$

that is,

$$L(w, b, \lambda, \mu) = \frac{1}{2} \begin{pmatrix} w^\top & b \end{pmatrix} \begin{pmatrix} I_n & 0_n \\ 0_n & 0 \end{pmatrix} \begin{pmatrix} w \\ b \end{pmatrix} + \begin{pmatrix} w^\top & b \end{pmatrix} \begin{pmatrix} X \begin{pmatrix} \lambda \\ \mu \end{pmatrix} \\ 1_p \lambda - 1_q \mu \end{pmatrix} + \begin{pmatrix} \lambda^\top & \mu^\top \end{pmatrix} \begin{pmatrix} 1_p + 1_q \end{pmatrix},$$

**Step 4:** Find the dual function $G(\lambda, \mu)$.

In order to find the dual function $G(\lambda, \mu)$ we need to minimize $L(w, b, \lambda, \mu)$ with respect to $w$ and $b$ and for this, since the objective function $J$ is convex and since $\mathbb{R}^{n+1}$ is convex and open, we can apply Theorem 21.11, which gives a necessary and sufficient condition for a minimum. The gradient of $L(w, b, \lambda, \mu)$ with respect to $w$ and $b$ is

$$\nabla L_{w,b} = \begin{pmatrix} I_n & 0_n \\ 0_n & 0 \end{pmatrix} \begin{pmatrix} w \\ b \end{pmatrix} + \begin{pmatrix} X \begin{pmatrix} \lambda \\ \mu \end{pmatrix} \\ 1_p \lambda - 1_q \mu \end{pmatrix} = \begin{pmatrix} w \\ 0 \end{pmatrix} + \begin{pmatrix} X \begin{pmatrix} \lambda \\ \mu \end{pmatrix} \\ 1_p^\top \lambda - 1_q^\top \mu \end{pmatrix}.$$ 

The necessary and sufficient condition for a minimum is

$$\nabla L_{w,b} = 0,$$

which yields

$$w = -X \begin{pmatrix} \lambda \\ \mu \end{pmatrix} \quad \text{()} \quad \text{(}1\text{)}$$

and

$$1_p^\top \lambda - 1_q^\top \mu = 0. \quad \text{(}2\text{)}$$
The second equation can be written as
\[
\sum_{i=1}^{p} \lambda_i = \sum_{j=1}^{q} \mu_j. \tag{3.3}
\]
Plugging back \( w \) from (3.1) into the Lagrangian and using (3.2) we get
\[
G(\lambda, \mu) = -\frac{1}{2} (\lambda^T \mu^T) X^T X \left(\begin{array}{c} \lambda \\ \mu \end{array}\right) + (\lambda^T \mu^T) \mathbf{1}_{p+q}; \tag{3.4}
\]
of course, \((\lambda^T \mu^T) \mathbf{1}_{p+q} = \sum_{i=1}^{p} \lambda_i + \sum_{j=1}^{q} \mu_j\). Actually, to be perfectly rigorous \(G(\lambda, \mu)\) is only defined on the intersection of the hyperplane of equation \(\sum_{i=1}^{p} \lambda_i = \sum_{j=1}^{q} \mu_j\) with the convex octant in \(\mathbb{R}^{p+1}\) given by \(\lambda \geq 0, \mu \geq 0\), so for all \(\lambda \in \mathbb{R}^{p}_{+}\) and all \(\mu \in \mathbb{R}^{q}_{+}\), we have
\[
G(\lambda, \mu) = \begin{cases} 
-\frac{1}{2} (\lambda^T \mu^T) X^T X \left(\begin{array}{c} \lambda \\ \mu \end{array}\right) + (\lambda^T \mu^T) \mathbf{1}_{p+q} & \text{if } \sum_{i=1}^{p} \lambda_i = \sum_{j=1}^{q} \mu_j \\
-\infty & \text{otherwise.}
\end{cases}
\]

Note that the condition
\[
\sum_{i=1}^{p} \lambda_i = \sum_{j=1}^{q} \mu_j
\]
is Condition (3.2) of Example 31.4, which is not surprising.

**Step 5:** Write the dual program in matrix form.

Maximizing the dual function \(G(\lambda, \mu)\) over its domain of definition is equivalent to maximizing
\[
\tilde{G}(\lambda, \mu) = -\frac{1}{2} (\lambda^T \mu^T) X^T X \left(\begin{array}{c} \lambda \\ \mu \end{array}\right) + (\lambda^T \mu^T) \mathbf{1}_{p+q}
\]
subject to the constraint
\[
\sum_{i=1}^{p} \lambda_i = \sum_{j=1}^{q} \mu_j,
\]
so we formulate the dual program as,
\[
\text{maximize} \quad -\frac{1}{2} (\lambda^T \mu^T) X^T X \left(\begin{array}{c} \lambda \\ \mu \end{array}\right) + (\lambda^T \mu^T) \mathbf{1}_{p+q}
\]
subject to
\[
\sum_{i=1}^{p} \lambda_i = \sum_{j=1}^{q} \mu_j \\
\lambda \geq 0, \mu \geq 0,
\]
or equivalently,

\[
\begin{align*}
\text{minimize} & \quad \frac{1}{2} (\lambda^\top \mu^\top) X^\top X \begin{pmatrix} \lambda \\ \mu \end{pmatrix} - (\lambda^\top \mu^\top) 1_{p+q} \\
\text{subject to} & \quad \sum_{i=1}^p \lambda_i = \sum_{j=1}^q \mu_j \\
& \quad \lambda \geq 0, \mu \geq 0.
\end{align*}
\]

The constraints of the dual program are a lot simpler than the constraints

\[
\begin{pmatrix} X^\top 1_p \\ -1_q \end{pmatrix} \begin{pmatrix} w \\ b \end{pmatrix} \leq -1_{p+q}
\]

of the primal program because these constraints have been “absorbed” by the objective function \( \hat{G}(\lambda, \nu) \) of the dual program which involves the matrix \( X^\top X \). The matrix \( X^\top X \) is symmetric positive semidefinite, but not invertible in general.

**Step 6:** Solve the dual program.

This step involves using numerical procedures typically based on gradient descent to find \( \lambda \) and \( \mu \). Once \( \lambda \) and \( \mu \) are determined, \( w \) is determined by \((\ast_1)\) and \( b \) is determined as in Section 31.4 using the fact that there is at least some \( i_0 \) such that \( \lambda_{i_0} > 0 \) and some \( j_0 \) such that \( \mu_{j_0} > 0 \).

**Remarks:**

(1) Since the constraints are affine and the objective function is convex, by Theorem 31.16(2) the duality gap is zero, so for any minimum \( w \) of \( J(w, b) = (1/2)w^\top w \) and any maximum \((\lambda, \mu)\) of \( G \), we have

\[
J(w, b) = \frac{1}{2} w^\top w = G(\lambda, \mu).
\]

But by \((\ast_1)\)

\[
w = -X \begin{pmatrix} \lambda \\ \mu \end{pmatrix} = \sum_{i=1}^p \lambda_i u_i - \sum_{j=1}^q \mu_j v_j,
\]

so

\[
(\lambda^\top \mu^\top) X^\top X \begin{pmatrix} \lambda \\ \mu \end{pmatrix} = w^\top w,
\]

and we get

\[
\frac{1}{2} w^\top w = -\frac{1}{2} (\lambda^\top \mu^\top) X^\top X \begin{pmatrix} \lambda \\ \mu \end{pmatrix} + (\lambda^\top \mu^\top) 1_{p+q} = -\frac{1}{2} w^\top w + (\lambda^\top \mu^\top) 1_{p+q}.
\]
so

\[ w^\top w = (\lambda^\top \mu^\top) 1_{p+q} = \sum_{i=1}^{p} \lambda_i + \sum_{j=1}^{q} \mu_j, \]

which yields

\[ G(\lambda, \mu) = \frac{1}{2} \left( \sum_{i=1}^{p} \lambda_i + \sum_{j=1}^{q} \mu_j \right). \]

The above formulae are stated in Vapnik [111] (Chapter 10, Section 1).

(2) It is instructive to compute the Lagrangian of the dual program and to derive the KKT conditions for this Lagrangian.

The conditions \( \lambda \geq 0 \) being equivalent to \( -\lambda \leq 0 \), and the conditions \( \mu \geq 0 \) being equivalent to \( -\mu \leq 0 \), we introduce Lagrange multipliers \( \alpha \in \mathbb{R}^p_+ \) and \( \beta \in \mathbb{R}^q_+ \) as well as a multiplier \( \rho \in \mathbb{R} \) for the equational constraint, and we form the Lagrangian

\[
L(\lambda, \mu, \alpha, \beta, \rho) = \frac{1}{2} (\lambda^\top \mu^\top) X^\top X \left( \begin{array}{c} \lambda \\ \mu \end{array} \right) - (\lambda^\top \mu^\top) 1_{p+q} \\
- \sum_{i=1}^{p} \alpha_i \lambda_i - \sum_{j=1}^{q} \beta_j \mu_j + \rho \left( \sum_{j=1}^{q} \mu_j - \sum_{i=1}^{p} \lambda_i \right).
\]

It follows that the KKT conditions are

\[
X^\top X \left( \begin{array}{c} \lambda \\ \mu \end{array} \right) - 1_{p+q} - \left( \begin{array}{c} \alpha \\ \beta \end{array} \right) + \rho \left( \begin{array}{c} -1_{p} \\ -1_{q} \end{array} \right) = 0_{p+q}, \tag{*4}
\]

and \( \alpha_i \lambda_i = 0 \) for \( i = 1, \ldots, p \) and \( \beta_j \mu_j = 0 \) for \( j = 1, \ldots, q \).

But (*4) is equivalent to

\[
-X^\top X \left( \begin{array}{c} \lambda \\ \mu \end{array} \right) + \rho \left( \begin{array}{c} 1_{p} \\ -1_{q} \end{array} \right) + 1_{p+q} + \left( \begin{array}{c} \alpha \\ \beta \end{array} \right) = 0_{p+q},
\]

which is precisely the result of adding \( \alpha \geq 0 \) and \( \beta \geq 0 \) as slack variables to the inequalities (*3) of Example 31.4, namely

\[
-X^\top X \left( \begin{array}{c} \lambda \\ \mu \end{array} \right) + b \left( \begin{array}{c} 1_{p} \\ -1_{q} \end{array} \right) + 1_{p+q} \leq 0_{p+q},
\]

to make them equalities, where \( \rho \) plays the role of \( b \).

When the constraints are affine, the dual function \( G(\lambda, \nu) \) can be expressed in terms of the conjugate of the objective function \( J \).
14.7 Conjugate Function and Legendre Dual Function

The notion of conjugate function goes back to Legendre and plays an important role in classical mechanics for converting a Lagrangian to a Hamiltonian; see Arnold [4] (Chapter 3, Sections 14 and 15).

Definition 14.10. Let \( f : A \to \mathbb{R} \) be a function defined on some subset \( A \) of \( \mathbb{R}^n \). The conjugate \( f^* \) of the function \( f \) is the partial function \( f^* : \mathbb{R}^n \to \mathbb{R} \) defined by

\[
f^*(y) = \sup_{x \in A} (y^\top x - f(x)), \quad y \in \mathbb{R}^n.
\]

The conjugate of a function is also called the Fenchel conjugate, or Legendre transform when \( f \) is differentiable.

As the pointwise supremum of a family of affine functions in \( y \), the conjugate function \( f^* \) is convex, even if the original function \( f \) is not convex.

The domain of \( f^* \) can be very small, even if the domain of \( f \) is big. For example, if \( f : \mathbb{R} \to \mathbb{R} \) is the affine function given by \( f(x) = ax + b \) (with \( a, b \in \mathbb{R} \)), then the function \( x \mapsto yx - ax - b \) is unbounded above unless \( y = a \), so

\[
f^*(y) = \begin{cases} 
  -b & \text{if } y = a \\
  +\infty & \text{otherwise}.
\end{cases}
\]

The domain of \( f^* \) can also be bigger than the domain of \( f \); see Example 31.9(3).

The conjugate of many functions that come up in optimization are derived in Boyd and Vandenberghe; see [22], Section 3.3. We mention a few that will be used in this chapter.

Example 14.9.

1. **Negative logarithm**: \( f(x) = -\log x \), with \( \text{dom}(f) = \{ x \in \mathbb{R} \mid x > 0 \} \). The function \( x \mapsto yx + \log x \) is unbounded above if \( y \geq 0 \), and when \( y < 0 \), its maximum is obtained iff its derivative is zero, namely

\[
y + \frac{1}{x} = 0.
\]

Substituting for \( x = -1/y \) in \( yx + \log x \), we obtain \(-1 + \log(-1/y) = -1 - \log(-y)\), so we have

\[
f^*(y) = -\log(-y) - 1,
\]

with \( \text{dom}(f^*) = \{ y \in \mathbb{R} \mid y < 0 \} \).

2. **Exponential**: \( f(x) = e^x \), with \( \text{dom}(f) = \mathbb{R} \). The function \( x \mapsto yx - e^x \) is unbounded if \( y < 0 \). When \( y > 0 \), it reaches a maximum iff its derivative is zero, namely

\[
y - e^x = 0.
\]
Substituting for $x = \log y$ in $yx - e^x$, we obtain $y \log y - y$, so we have
\[ f^*(y) = y \log y - y, \]
with $\text{dom}(f^*) = \{ y \in \mathbb{R} \mid y \geq 0 \}$, with the convention that $0 \log 0 = 0$.

(3) **Negative Entropy**: $f(x) = x \log x$, with $\text{dom}(f) = \{ x \in \mathbb{R} \mid x \geq 0 \}$, with the convention that $0 \log 0 = 0$. The function $x \mapsto yx - x \log x$ is bounded above for all $y > 0$, and it attains its maximum when its derivative is zero, namely
\[ y - \log x - 1 = 0. \]
Substituting for $x = e^{y-1}$ in $yx - x \log x$, we obtain $ye^{y-1} - e^{y-1}(y - 1) = e^{y-1}$, which yields
\[ f^*(y) = e^{y-1}, \]
with $\text{dom}(f) = \mathbb{R}$.

(4) **Strictly convex quadratic function**: $f(x) = \frac{1}{2} x^\top Ax$, where $A$ is an $n \times n$ symmetric positive definite matrix, with $\text{dom}(f) = \mathbb{R}^n$. The function $x \mapsto y^\top x - \frac{1}{2} x^\top Ax$ has a unique minimum when its gradient is zero, namely
\[ y = Ax. \]
Substituting for $x = A^{-1}y$ in $y^\top x - \frac{1}{2} x^\top Ax$, we obtain
\[ y^\top A^{-1}y - \frac{1}{2} y^\top A^{-1}y = -\frac{1}{2} y^\top A^{-1}y, \]
so
\[ f^*(y) = -\frac{1}{2} y^\top A^{-1}y \]
with $\text{dom}(f^*) = \mathbb{R}^n$.

(5) **Log-determinant**: $f(X) = \log \det(X^{-1})$, where $X$ is an $n \times n$ symmetric positive definite matrix. Then
\[ f(Y) = \log \det((-Y)^{-1}) - n, \]
where $Y$ is an $n \times n$ symmetric negative definite matrix; see Boyd and Vandenberghe; see [22], Section 3.3.1, Example 3.23.

(6) **Norm on $\mathbb{R}^n$**: $f(x) = \|x\|$ for any norm $\|\|$ on $\mathbb{R}^n$, with $\text{dom}(f) = \mathbb{R}^n$. Recall from Section 12.6 that the dual norm $\|\|^D$ of the norm $\|$ (with respect to the canonical inner product $x \cdot y = y^\top x$ on $\mathbb{R}^n$ is given by
\[ \|y\|^D = \sup_{\|x\| = 1} |y^\top x|, \]
and that
\[ |y^\top x| \leq \|x\| \|y\|^D. \]

We have
\[
    f^*(y) = \sup_{x \in \mathbb{R}^n} (y^\top x - \|x\|)
    = \sup_{x \in \mathbb{R}^n, x \neq 0} \left( y^\top \frac{x}{\|x\|} - 1 \right) \|x\|
    \leq \sup_{x \in \mathbb{R}^n, x \neq 0} (\|y\|^D - 1) \|x\|,
\]
so if \(\|y\|^D > 1\) this last term goes to \(+\infty\), but if \(\|y\|^D \leq 1\), then its maximum is 0. Therefore,
\[
f^*(y) = \|y\|^* = \begin{cases} 0 & \text{if } \|y\|^D \leq 1 \\ +\infty & \text{otherwise.} \end{cases}
\]

(7) **Norm squared:** \(f(x) = \frac{1}{2} \|x\|^2\) for any norm \(\|\|\) on \(\mathbb{R}^n\), with \(\text{dom}(f) = \mathbb{R}^n\). Since \(|y^\top x| \leq \|x\| \|y\|^D\), we have
\[
y^\top x - (1/2) \|x\|^2 \leq \|y\|^D \|x\| - (1/2) \|x\|^2.
\]
The right-hand side is a quadratic function of \(\|x\|\) which achieves its maximum at \(\|x\| = \|y\|^D\), with maximum value \((1/2)(\|y\|^D)^2\). Therefore
\[
y^\top x - (1/2) \|x\|^2 \leq (1/2) \left(\|y\|^D\right)^2
\]
for all \(x\), which shows that
\[
f^*(y) \leq \left(1/2\right) \left(\|y\|^D\right)^2.
\]
By definition of the dual norm and because the unit sphere is compact, for any \(y \in \mathbb{R}^n\) there is some \(x \in \mathbb{R}^n\) such that \(\|x\| = 1\) and \(y^\top x = \|y\|^D\), so multiplying both sides by \(\|y\|^D\) we obtain
\[
y^\top \|y\|^D x = \left(\|y\|^D\right)^2
\]
and for \(z = \|y\|^D x\), since \(\|x\| = 1\) we have \(\|z\| = \|y\|^D \|x\| = \|y\|^D\), so we get
\[
y^\top z - (1/2)(\|z\|^2) = \left(\|y\|^D\right)^2 - (1/2) \left(\|y\|^D\right)^2 = (1/2) \left(\|y\|^D\right)^2,
\]
which shows that the upper bound \((1/2) \left(\|y\|^D\right)^2\) is achieved. Therefore,
\[
f^*(y) = \frac{1}{2} \left(\|y\|^D\right)^2,
\]
and \(\text{dom}(f^*) = \mathbb{R}^n\).
(8) Log-sum-exp function: \( f(x) = \log \left( \sum_{i=1}^{n} e^{x_i} \right) \), where \( x = (x_1, \ldots, x_n) \in \mathbb{R}^n \). To determine the values of \( y \in \mathbb{R}^n \) for which the maximum of \( g(x) = y^\top x - f(x) \) over \( x \in \mathbb{R}^n \) is attained, we compute its gradient and we find

\[
\nabla g_x = \begin{pmatrix}
y_1 - \frac{e^{x_1}}{\sum_{i=1}^{n} e^{x_i}} \\
\vdots \\
y_n - \frac{e^{x_n}}{\sum_{i=1}^{n} e^{x_i}}
\end{pmatrix}.
\]

Therefore, \((y_1, \ldots, y_n)\) must satisfy the system of equations

\[
y_j = \frac{e^{x_j}}{\sum_{i=1}^{n} e^{x_i}}, \quad j = 1, \ldots, n. \tag{*}
\]

The condition \( \sum_{i=1}^{n} y_i = 1 \) is obviously necessary, as well as the conditions \( y_i > 0 \), for \( i = 1, \ldots, n \). Conversely, if \( 1^\top y = 1 \) and \( y > 0 \), then \( x_j = \log y_i \) for \( i = 1, \ldots, n \) is a solution. Since (*) implies that

\[
x_i = \log y_i + \log \left( \sum_{i=1}^{n} e^{x_i} \right), \tag{**}
\]

we get

\[
y^\top x - f(x) = \sum_{i=1}^{n} y_i x_i - \log \left( \sum_{i=1}^{n} e^{x_i} \right) \\
= \sum_{i=1}^{n} y_i \log y_i + \sum_{i=1}^{n} y_i \log \left( \sum_{i=1}^{n} e^{x_i} \right) - \log \left( \sum_{i=1}^{n} e^{x_i} \right) \text{ by (**)} \\
= \sum_{i=1}^{n} y_i \log y_i + \left( \sum_{i=1}^{n} y_i - 1 \right) \log \left( \sum_{i=1}^{n} e^{x_i} \right) \\
= \sum_{i=1}^{n} y_i \log y_i \text{ since } \sum_{i=1}^{n} y_i = 1.
\]

Consequently, if \( f^*(y) \) is defined, then \( f^*(y) = \sum_{i=1}^{n} y_i \log y_i \). If we agree that \( 0 \log 0 = 0 \), then it is an easy exercise (or, see Boyd and Vandenberghe [22], Section 3.3, Example 3.25) to show that

\[
f^*(y) = \begin{cases} 
\sum_{i=1}^{n} y_i \log y_i & \text{if } 1^\top y = 1 \text{ and } y \geq 0 \\
\infty & \text{otherwise}.
\end{cases}
\]

Thus we obtain the negative entropy restricted to the domain \( 1^\top y = 1 \) and \( y \geq 0 \).
By definition of \( f^* \) we have
\[
f(x) + f^*(y) \geq x^T y,
\]
whenever the left-hand side is defined. The above is known as Fenchel’s inequality (or Young’s inequality if \( f \) is differentiable).

If \( f : A \to \mathbb{R} \) is convex (so \( A \) is convex) and if \( \text{epi}(f) \) is closed, then it can be shown that \( f^{**} = f \). In particular, this is true if \( A = \mathbb{R}^n \).

If \( f : \mathbb{R}^n \to \mathbb{R} \) is convex and differentiable, then \( x^* \) maximizes \( x^T y - f(x) \) iff \( x^* \) minimizes \( -x^T y + f(x) \) iff
\[
\nabla f_{x^*} = y,
\]
and so
\[
f^*(y) = (x^*)^T \nabla f_{x^*} - f(x^*).
\]
Consequently, if we can solve the equation
\[
\nabla f_z = y
\]
for \( z \) given \( y \), then we obtain \( f^*(y) \).

It can be shown that if \( f \) is twice differentiable, strictly convex, and surlinear, which means that
\[
\lim_{\|y\| \to +\infty} \frac{f(y)}{\|y\|} = +\infty,
\]
then there is a unique \( x_y \) such that \( \nabla f_{x_y} = y \), so that
\[
f^*(y) = x_y^T \nabla f_{x_y} - f(x_y),
\]
and \( f^* \) is differentiable with
\[
\nabla f^*_y = x_y.
\]

We now return to our optimization problem.

**Proposition 14.17.** Consider the problem \((P)\),

\[
\text{minimize} \quad J(v) \\
\text{subject to} \quad Av \leq b \\
\quad \quad Cv = d,
\]

with affine inequality and equality constraints (with \( A \) an \( m \times n \) matrix, \( C \) an \( p \times n \) matrix, \( b \in \mathbb{R}^m \), \( d \in \mathbb{R}^p \)). The dual function \( G(\lambda, \nu) \) is given by
\[
G(\lambda, \nu) = \begin{cases} 
-b^T \lambda - d^T \nu - J^*(-A^T \lambda - C^T \nu) & \text{if } -A^T \lambda - C^T \nu \in \text{dom}(J^*), \\
-\infty & \text{otherwise},
\end{cases}
\]
for all \( \lambda \in \mathbb{R}_+^m \) and all \( \nu \in \mathbb{R}^p \), where \( J^* \) is the conjugate of \( J \).
Proof. The Lagrangian associated with the above program is

\[ L(v, \lambda, \nu) = J(v) + (Av - b)^\top \lambda + (Cv - d)^\top \nu \]

\[ = -b^\top \lambda - d^\top \nu + J(v) + (A^\top \lambda + C^\top \nu)^\top v, \]

with \( \lambda \in \mathbb{R}^m_+ \) and \( \nu \in \mathbb{R}^p \). By definition

\[ G(\lambda, \nu) = -b^\top \lambda - d^\top \nu + \inf_{v \in \mathbb{R}^n} (J(v) + (A^\top \lambda + C^\top \nu)^\top v) \]

\[ = -b^\top \lambda - d^\top \nu + \sup_{v \in \mathbb{R}^n} (- (A^\top \lambda + C^\top \nu)^\top v - J(v)) \]

\[ = -b^\top \lambda - d^\top \nu - J^*( -A^\top \lambda - C^\top \nu). \]

Therefore, for all \( \lambda \in \mathbb{R}^m_+ \) and all \( \nu \in \mathbb{R}^p \), we have

\[ G(\lambda, \nu) = \begin{cases} 
-b^\top \lambda - d^\top \nu - J^*( -A^\top \lambda - C^\top \nu) & \text{if } -A^\top \lambda - C^\top \nu \in \text{dom}(J^*), \\
-\infty & \text{otherwise},
\end{cases} \]

as claimed.

As application of this result, consider the following example.

**Example 14.10.** Consider the following problem:

\[ \underset{v}{\text{minimize}} \quad \|v\| \]

\[ \text{subject to} \quad Av = b, \]

where \( \| \cdot \| \) is any norm on \( \mathbb{R}^n \). Using the result of Example 31.9, we obtain

\[ G(\nu) = -b^\top \nu - \| -A^\top \nu \|^*, \]

that is,

\[ G(\nu) = \begin{cases} 
-b^\top \nu & \text{if } \|A^\top \nu\|^D \leq 1 \\
-\infty & \text{otherwise}.
\end{cases} \]

In the special case where \( \| \cdot \| = \| \cdot \|_2 \), we also have \( \| \cdot \|^D = \| \cdot \|_2 \).

Another interesting application is to the entropy minimization problem.

**Example 14.11.** Consider the following problem known as entropy minimization:

\[ \underset{x}{\text{minimize}} \quad f(x) = \sum_{i=1}^n x_i \log x_i \]

\[ \text{subject to} \quad Ax \leq b \]

\[ 1^\top x = 1, \]
where \( \text{dom}(f) = \{ x \in \mathbb{R}^n \mid x \geq 0 \} \). By Example 31.9(3), the conjugate of the negative entropy function \( u \log u \) is \( e^{u-1} \), so we easily see that

\[
f^*(y) = \sum_{i=1}^{n} e^{y_i-1},
\]

which is defined on \( \mathbb{R}^n \). Using our above result, the dual function \( G(\lambda, \mu) \) of the entropy minimization problem is given by

\[
G(\lambda, \mu) = -b^\top \lambda - \mu - e^{-\mu-1} \sum_{i=1}^{n} e^{-(A_i^\top) \lambda},
\]

for all \( \lambda \in \mathbb{R}_+^n \) and all \( \mu \in \mathbb{R} \), where \( A_i \) is the \( i \)th column of \( A \). It follows that the dual program is:

\[
\begin{align*}
\text{maximize} & \quad -b^\top \lambda - \mu - e^{-\mu-1} \sum_{i=1}^{n} e^{-(A_i^\top) \lambda} \\
\text{subject to} & \quad \lambda \geq 0.
\end{align*}
\]

We can simplify this problem by maximizing over the variable \( \mu \in \mathbb{R} \). For fixed \( \lambda \), the objective function is maximized when the derivative is zero, that is,

\[
-1 + e^{-\mu-1} \sum_{i=1}^{n} e^{-(A_i^\top) \lambda} = 0,
\]

which yields

\[
\mu = \log \left( \sum_{i=1}^{n} e^{-(A_i^\top) \lambda} \right) - 1.
\]

Plugging the above value back into the objective function of the dual we obtain the following program:

\[
\begin{align*}
\text{maximize} & \quad -b^\top \lambda - \log \left( \sum_{i=1}^{n} e^{-(A_i^\top) \lambda} \right) \\
\text{subject to} & \quad \lambda \geq 0.
\end{align*}
\]

The entropy minimization problem is another problem for which Theorem 31.15 applies, and thus can be solved using the dual program. Indeed, the Lagrangian of the primal program is given by

\[
L(x, \lambda, \mu) = \sum_{i=1}^{n} x_i \log x_i + \lambda^\top (Ax - b) + \mu(1^\top x - 1).
\]
Using the second derivative criterion for convexity, we see that \( L(x, \lambda, \mu) \) is strictly convex for \( x \in \mathbb{R}^n_+ \) and is bounded below, so it has a unique minimum which is obtained by setting the Laplacian \( \nabla L_x \) to zero. We have

\[
\nabla L_x = \begin{pmatrix}
\log x_1 + 1 + (A^1)^\top \lambda + \mu \\
\vdots \\
\log x_n + 1 + (A^n)^\top \lambda + \mu
\end{pmatrix}
\]

so by setting \( \nabla L_x \) to 0 we obtain

\[
x_i = e^{-(A^n)^\top \lambda + \mu + 1}, \quad i = 1, \ldots, n.
\] (*

By Theorem 31.15, since the objective function is convex and the constraints are affine, if the primal has a solution then so does the dual, and \( \lambda \) and \( \mu \) constitute an optimal solution of the dual, then \( x = (x_1, \ldots, x_n) \) given by the equations in (*) is an optimal solution of the primal.

Other examples are given in Boyd and Vandenberghe; see [22], Section 5.1.6.

The derivation of the dual function of Problem (SVM\(_{h1}\)) from Section 31.3 involves a similar type of reasoning.

**Example 14.12.** Consider the hard margin Problem (SVM\(_{h1}\)):

\[
\text{maximize} \quad \delta \\
\text{subject to} \\
w^\top u_i - b \geq \delta \quad i = 1, \ldots, p \\
-w^\top v_j + b \geq \delta \quad j = 1, \ldots, q \\
\|w\|_2 \leq 1,
\]

which is converted to the following minimization problem:

\[
\text{minimize} \quad -2\delta \\
\text{subject to} \\
w^\top u_i - b \geq \delta \quad i = 1, \ldots, p \\
-w^\top v_j + b \geq \delta \quad j = 1, \ldots, q \\
\|w\|_2 \leq 1,
\]

We replaced \( \delta \) by \( 2\delta \) because this will make it easier to find a nice geometric interpretation. Recall from Section 31.3 that Problem (SVM\(_{h1}\)) has a an optimal solution iff \( \delta > 0 \), in which case \( \|w\| = 1 \).
The corresponding Lagrangian with \( \lambda \in \mathbb{R}^p_+, \mu \in \mathbb{R}^q_+, \gamma \in \mathbb{R}^+ \), is

\[
L(w, b, \delta, \lambda, \mu, \gamma) = -2\delta + \sum_{i=1}^{p} \lambda_i (\delta + b - w^\top u_i) + \sum_{j=1}^{q} \mu_j (\delta - b + w^\top v_j) + \gamma (\|w\|_2 - 1)
\]

\[
= w^\top \left( -\sum_{i=1}^{p} \lambda_i u_i + \sum_{j=1}^{q} \mu_j v_j \right) + \gamma \|w\|_2 + \left( \sum_{i=1}^{p} \lambda_i - \sum_{j=1}^{q} \mu_j \right) b
\]

\[
+ \left( -2 + \sum_{i=1}^{p} \lambda_i + \sum_{j=1}^{q} \mu_j \right) \delta - \gamma.
\]

Next to find the dual function \( G(\lambda, \mu, \gamma) \) we need to minimize \( L(w, b, \delta, \lambda, \mu, \gamma) \) with respect to \( w, b \) and \( \delta \), so its gradient with respect to \( w, b \) and \( \delta \) must be zero. This implies that

\[
\sum_{i=1}^{p} \lambda_i - \sum_{j=1}^{q} \mu_j = 0
\]

\[
-2 + \sum_{i=1}^{p} \lambda_i + \sum_{j=1}^{q} \mu_j = 0,
\]

which yields

\[
\sum_{i=1}^{p} \lambda_i = \sum_{j=1}^{q} \mu_j = 1.
\]

Our minimization problem is reduced to: find

\[
\inf_{w, \|w\| \leq 1} \left( w^\top \left( \sum_{j=1}^{q} \mu_j v_j - \sum_{i=1}^{p} \lambda_i u_i \right) + \gamma \|w\|_2 - \gamma \right)
\]

\[
= -\gamma - \gamma \inf_{w, \|w\| \leq 1} \left( -w^\top \frac{1}{\gamma} \left( \sum_{j=1}^{q} \mu_j v_j - \sum_{i=1}^{p} \lambda_i u_i \right) + \|w\|_2 \right)
\]

\[
= \begin{cases} 
-\gamma & \text{if } \left\| \frac{1}{\gamma} \left( \sum_{j=1}^{q} \mu_j v_j - \sum_{i=1}^{p} \lambda_i u_i \right) \right\|_2 \leq 1 \\
-\infty & \text{otherwise}
\end{cases}
\]

by definition of \( \| \|_2^* \)

\[
= \begin{cases} 
-\gamma & \text{if } \left\| \sum_{j=1}^{q} \mu_j v_j - \sum_{i=1}^{p} \lambda_i u_i \right\|_2 \leq \gamma \\
-\infty & \text{otherwise}
\end{cases}
\]

since \( \| \|_2^* = \| \|_2 \) and \( \gamma > 0 \)

It is immediately verified that the above formula is still correct if \( \gamma = 0 \). Therefore

\[
G(\lambda, \mu, \gamma) = \begin{cases} 
-\gamma & \text{if } \left\| \sum_{j=1}^{q} \mu_j v_j - \sum_{i=1}^{p} \lambda_i u_i \right\|_2 \leq \gamma \\
-\infty & \text{otherwise}
\end{cases}
\]
CHAPTER 14. INTRODUCTION TO NONLINEAR OPTIMIZATION

Since \( \| \sum_{j=1}^{q} \mu_j v_j - \sum_{i=1}^{p} \lambda_i u_i \|_2 \leq \gamma \) iff \( -\gamma \leq -\| \sum_{j=1}^{q} \mu_j v_j - \sum_{i=1}^{p} \lambda_i u_i \|_2 \), the dual program, maximizing \( G(\lambda, \mu, \gamma) \), is equivalent to

\[
\text{maximize} \quad -\| \sum_{j=1}^{q} \mu_j v_j - \sum_{i=1}^{p} \lambda_i u_i \|_2
\]

subject to

\[
\sum_{i=1}^{p} \lambda_i = 1, \quad \lambda \geq 0
\]

\[
\sum_{j=1}^{q} \mu_j = 1, \quad \mu \geq 0,
\]
equivalently

\[
\text{minimize} \quad \| \sum_{j=1}^{q} \mu_j v_j - \sum_{i=1}^{p} \lambda_i u_i \|_2
\]

subject to

\[
\sum_{i=1}^{p} \lambda_i = 1, \quad \lambda \geq 0
\]

\[
\sum_{j=1}^{q} \mu_j = 1, \quad \mu \geq 0.
\]

Geometrically, \( \sum_{i=1}^{p} \lambda_i u_i \) with \( \sum_{i=1}^{p} \lambda_i = 1 \) and \( \lambda \geq 0 \) is a convex combinations of the \( u_i \)'s, and \( \sum_{j=1}^{q} \mu_j v_j \) with \( \sum_{j=1}^{q} \mu_j = 1 \) and \( \mu \geq 0 \) is a convex combination of the \( v_j \)'s, so the dual program is to minimize the distance between the polyhedron \( \text{conv}(u_1, \ldots, u_p) \) (the convex hull of the \( u_i \)'s) and the polyhedron \( \text{conv}(v_1, \ldots, v_q) \) (the convex hull of the \( v_j \)'s). Since both polyhedra are compact, the shortest distance between them is achieved. In fact, there is some vertex \( u_i \) such that if \( P(u_i) \) is its projection onto \( \text{conv}(v_1, \ldots, v_q) \) (which exists by Hilbert space theory), then the length of the line segment \( (u_i, P(u_i)) \) is the shortest distance between the two polyhedra (and similarly there is some vertex \( v_j \) such that if \( P(v_j) \) is its projection onto \( \text{conv}(u_1, \ldots, u_p) \) then the length of the line segment \( (v_j, P(v_j)) \) is the shortest distance between the two polyhedra).

If the two subsets are separable, in which case Problem (\text{SVM}_{\lambda_1}) has an optimal solution \( \delta > 0 \), because the objective function is convex and the convex constraint \( \| w \|_2 \leq 1 \) is qualified since \( \delta \) may be negative, by Theorem 31.14(2) the duality gap is zero, so \( \delta \) is half of the minimum distance between the two convex polyhedra \( \text{conv}(u_1, \ldots, u_p) \) and \( \text{conv}(v_1, \ldots, v_q) \); see Figure 31.19.

It should be noted that the constraint \( \| w \| \leq 1 \) yields a formulation of the dual problem which has the advantage of having a nice geometric interpretation: finding the minimal
Figure 14.19: In \( \mathbb{R}^2 \) the convex hull of the \( u_i \)'s, namely the blue hexagon, is separated from the convex hull of the \( v_j \)'s, i.e. the red square, by the purple hyperplane (line) which is the perpendicular bisector to the blue line segment between \( u_i \) and \( v_1 \), where this blue line segment is the shortest distance between the two convex polygons.

The distance between the convex polyhedra \( \text{conv}(u_1, \ldots, u_p) \) and \( \text{conv}(v_1, \ldots, v_q) \). Unfortunately this formulation is not useful for actually solving the problem. However, if the equivalent constraint \( \|w\|^2 (= w^\top w) \leq 1 \) is used, then the dual problem is much more useful as a solving tool.

In Chapter 34 we consider the case where the sets of points \( \{u_1, \ldots, u_p\} \) and \( \{v_1, \ldots, v_q\} \) are not linearly separable.

### 14.8 Some Techniques to Obtain a More Useful Dual Program

In some cases, it is advantageous to reformulate a primal optimization problem to obtain a more useful dual problem. Three different reformulations are proposed in Boyd and Vandenberghe; see [22], Section 5.7:

1. Introducing new variables and associated equality constraints.
2. Replacing the objective function with an increasing function of the original function.
3. Making explicit constraints implicit, that is, incorporating them into the domain of the objective function.

We only give illustrations of (1) and (2), and refer the reader to Boyd and Vandenberghe [22] (Section 5.7) for more examples of these techniques.
Consider the unconstrained program:

\[
\text{minimize } f(Ax + b),
\]

where \( A \) is an \( m \times n \) matrix and \( b \in \mathbb{R}^m \). While the conditions for a zero duality gap are satisfied, the Lagrangian is

\[
L(x) = f(Ax + b),
\]

so the dual function \( G \) is the constant function whose value is

\[
G = \inf_{x \in \mathbb{R}^n} f(Ax + b),
\]

which is not useful at all.

Let us reformulate the problem as

\[
\text{minimize } f(y)
\]

subject to

\[
Ax + b = y,
\]

where we introduced the new variable \( y \in \mathbb{R}^m \) and the equality constraint \( Ax + b = y \). The two problems are obviously equivalent. The Lagrangian of the reformulated problem is

\[
L(x, y, \mu) = f(y) + \mu^\top (Ax + b - y)
\]

where \( \mu \in \mathbb{R}^m \). To find the dual function \( G(\mu) \) we minimize \( L(x, y, \mu) \) over \( x \) and \( y \). Minimizing over \( x \) we see that \( G(\mu) = -\infty \) unless \( A^\top \mu = 0 \), in which case we are left with

\[
G(\mu) = b^\top \mu + \inf_y (f(y) - \mu^\top y) = b^\top \mu - \inf_y (\mu^\top y - f(y)) = b^\top \mu - f^*(\mu),
\]

where \( f^* \) is the conjugate of \( f \). It follows that the dual program can be expressed as

\[
\text{maximize } b^\top \mu - f^*(\mu)
\]

subject to

\[
A^\top \mu = 0.
\]

This formulation of the dual is much more useful than the dual of the original program.

**Example 14.13.** As a concrete example, consider the following unconstrained program:

\[
\text{minimize } f(x) = \log \left( \sum_{i=1}^{n} e^{(a^i)^\top x + b_i} \right)
\]
where $a^i$ is a column vector in $\mathbb{R}^n$. We reformulate the problem by introducing new variables and equality constraints as follows:

$$
\text{minimize} \quad f(y) = \log \left( \sum_{i=1}^{n} e^{y_i} \right)
$$

subject to

$$Ax + b = y,$$

where $A$ is the matrix whose columns are the vectors $a^i$ and $b = (b_1, \ldots, b_n)$. Since by Example 31.9(8) the conjugate of the log-sum-exp function $f(y) = \log \left( \sum_{i=1}^{n} e^{y_i} \right)$ is

$$f^*(\mu) = \begin{cases} 
\sum_{i=1}^{n} \mu_i \log \mu_i & \text{if } 1^\top \mu = 1 \text{ and } \mu \geq 0 \\
\infty & \text{otherwise},
\end{cases}$$

the dual of the reformulated problem can be expressed as

$$
\text{maximize} \quad b^\top \mu - \log \left( \sum_{i=1}^{n} \mu_i \log \mu_i \right)
$$

subject to

$$1^\top \mu = 1$$

$$A^\top \mu = 0$$

$$\mu \geq 0,$$

an entropy maximization problem.

**Example 14.14.** Similarly the unconstrained norm minimization problem

$$\text{minimize} \quad \|Ax - b\|,$$

where $\| \|$ is any norm on $\mathbb{R}^m$, has a dual function which is a constant, and is not useful. This problem can be reformulated as

$$\text{minimize} \quad \|y\|
$$

subject to

$$Ax - b = y.$$

By Example 31.9(6), the conjugate of the norm is given by

$$
\|y\|^* = \begin{cases} 
0 & \text{if } \|y\|^D \leq 1 \\
+\infty & \text{otherwise},
\end{cases}
$$
so the dual of the reformulated program is:

\[
\begin{align*}
\text{maximize} & \quad b^\top \mu \\
\text{subject to} & \quad \|\mu\|^{D} \leq 1 \\
& \quad A^\top \mu = 0.
\end{align*}
\]

Here is now an example of (2), replacing the objective function with an increasing function of the original function.

**Example 14.15.** The norm minimization of Example 31.14 can be reformulated as

\[
\begin{align*}
\text{minimize} & \quad \frac{1}{2} \|y\|^2 \\
\text{subject to} & \quad Ax - b = y.
\end{align*}
\]

This program is obviously equivalent to the original one. By Example 31.9(7), the conjugate of the square norm is given by

\[
\frac{1}{2} \left(\|y\|^D\right)^2,
\]

so the dual of the reformulated program is

\[
\begin{align*}
\text{maximize} & \quad -\frac{1}{2} \left(\|\mu\|^D\right)^2 + b^\top \mu \\
\text{subject to} & \quad A^\top \mu = 0.
\end{align*}
\]

Note that this dual is different from the dual obtained in Example 31.14.

The objective function of the dual program in Example 31.14 is linear, but we have the nonlinear constraint $\|\mu\|^D \leq 1$. On the other hand, the objective function of the dual program of Example 31.15 is quadratic, whereas its constraints are affine. We have other examples of this trade-off with the Programs (SVM$_{h2}$) (quadratic objective function, affine constraints), and (SVM$_{h1}$) (linear objective function, one nonlinear constraint).

Sometimes, it is also helpful to replace a constraint by an increasing function of this constraint; for example, to use the constraint $\|w\|_2^2 (= w^\top w) \leq 1$ instead of $\|w\|_2 \leq 1$.

In Chapter 32 we revisit the problem of solving an overdetermined or underdetermined linear system $Ax = b$ considered in Section 17.1 from a different point of view.
14.9 Uzawa’s Method

Let us go back to our minimization problem

\[
\begin{align*}
\text{minimize} & \quad J(v) \\
\text{subject to} & \quad \varphi_i(v) \leq 0, \quad i = 1, \ldots, m,
\end{align*}
\]

where the functions \( J \) and \( \varphi_i \) are defined on some open subset \( \Omega \) of a finite-dimensional Euclidean vector space \( V \) (more generally, a real Hilbert space \( V \)). As usual, let

\[ U = \{ v \in V \mid \varphi_i(v) \leq 0, \ 1 \leq i \leq m \}. \]

If the functional \( J \) satisfies the inequalities of Proposition 30.14 and if the functions \( \varphi_i \) are convex, in theory, the projected-gradient method converges to the unique minimizer of \( J \) over \( U \). Unfortunately, it is usually impossible to compute the projection map \( p_U : V \to U \).

On the other hand, the domain of the Lagrange dual function \( G : \mathbb{R}^m_+ \to \mathbb{R} \) given by

\[ G(\mu) = \inf_{v \in \Omega} L(v, \mu) \quad \mu \in \mathbb{R}^m_+, \]

is \( \mathbb{R}^m_+ \), where

\[ L(v, \mu) = J(v) + \sum_{i=1}^{m} \mu_i \varphi_i(v) \]

is the Lagrangian of our problem. Now the projection \( p_+ \) from \( \mathbb{R}^m \) to \( \mathbb{R}^m_+ \) is very simple, namely

\[ (p_+(\lambda))_i = \max\{\lambda_i, 0\}, \quad 1 \leq i \leq m. \]

It follows that the projection-gradient method should be applicable to the dual problem \( (D) \):

\[
\begin{align*}
\text{maximize} & \quad G(\mu) \\
\text{subject to} & \quad \mu \in \mathbb{R}^m_+.
\end{align*}
\]

If the hypotheses of Theorem 31.14 hold, then a solution \( \lambda \) of the dual program \( (D) \) yields a solution \( u_\lambda \) of the primal problem.

Uzawa’s method is essentially the gradient method with fixed stepsize applied to the dual problem \( (D) \). However, it is designed to yield a solution of the primal problem.

**Uzawa’s method:**

Given an arbitrary initial vectors \( \lambda^0 \in \mathbb{R}^m_+ \), two sequences \( (\lambda^k)_{k \geq 0} \) and \( (u^k)_{k \geq 0} \) are constructed, with \( \lambda^k \in \mathbb{R}^m_+ \) and \( u^k \in V \).

Assuming that \( \lambda^0, \lambda^1, \ldots, \lambda^k \) are known, \( u^k \) and \( \lambda^{k+1} \) are determined as follows:
$u^k$ is the unique solution of the minimization problem, find $u^k \in V$ such that

\[
(UZ) \quad \begin{cases}
J(u^k) + \sum_{i=1}^{m} \lambda^k_i \varphi_i(u^k) = \inf_{v \in V} \left( J(v) + \sum_{i=1}^{m} \lambda^k_i \varphi_i(v) \right); \text{ and }
\lambda^{k+1}_i = \max \{ \lambda^k_i + \rho \varphi_i(u^k), 0 \}, \quad 1 \leq i \leq m,
\end{cases}
\]

where $\rho > 0$ is a suitably chosen parameter.

Recall that the proof of Theorem 31.14 shows that

\[ G'_\lambda(\xi) = \langle \nabla G_\lambda, \xi \rangle = \sum_{i=1}^{m} \xi_i \varphi_i(u^k), \]

which means that $(\nabla G_\lambda)_i = \varphi_i(u^k)$. Then the second equation in $(UZ)$ corresponds to the gradient-projection step

\[ \lambda^{k+1}_i = p_+ (\lambda^k_i + \rho \nabla G_\lambda u^k). \]

Note that because the problem is a maximization problem we use a positive sign instead of a negative sign. Uzawa’s method is indeed a gradient method.

Basically, Uzawa’s method replaces a constrained optimization problem by a sequence of unconstrained optimization problems involving the Lagrangian of the (primal) problem.

Interestingly, under certain hypotheses, it is possible to prove that the sequence of approximate solutions $(u^k)_{k \geq 0}$ converges to the minimizer $u$ of $J$ over $U$, even if the sequence $(\lambda^k)_{k \geq 0}$ does not converge. We prove such a result when the constraints $\varphi_i$ are affine.

**Theorem 14.18.** Suppose $J: \mathbb{R}^n \to \mathbb{R}$ is an elliptic functional, which means that $J$ is continuously differentiable on $\mathbb{R}^n$, and there is some constant $\alpha > 0$ such that

\[ \langle \nabla J_v - \nabla J_u, v - u \rangle \geq \alpha \| v - u \|^2 \quad \text{for all } u, v \in V, \]

and that $U$ is a nonempty closed convex subset given by

\[ U = \{ v \in \mathbb{R}^n \mid Cv \leq d \}, \]

where $C$ is a real $m \times n$ matrix and $d \in \mathbb{R}^m$. If the scalar $\rho$ satisfies the condition

\[ 0 < \rho < \frac{2\alpha}{\| C \|_2^2}, \]

where $\| C \|_2$ is the spectral norm of $C$, then the sequence $(u^k)_{k \geq 0}$ computed by Uzawa’s method converges to the unique minimizer $u \in U$ of $J$.

Furthermore, if $C$ has rank $m$, then the sequence $(\lambda^k)_{k \geq 0}$ converges to the unique maximizer of the dual problem $(D)$. 
Proof.

Step 1. We establish algebraic conditions relating the unique minimizer \( u \in U \) of \( J \) over \( U \) and some \( \lambda \in \mathbb{R}_+^m \) such that \((u, \lambda)\) is a saddle point.

Since \( J \) is elliptic and \( U \) is nonempty closed and convex, by Theorem 30.7, the functional \( J \) is strictly convex, so it has a unique minimizer \( u \in U \). Since \( J \) is convex and the constraints are affine, by Theorem 31.14(2) the dual problem \((D)\) has at least one solution. By Theorem 31.12(2), there is some \( \lambda \in \mathbb{R}_+^m \) such that \((u, \lambda)\) is a saddle point of the Lagrangian \( L \).

If we define the affine function \( \varphi \) by

\[
\varphi(v) = (\varphi_1(v), \ldots, \varphi_m(v)) = Cv - d,
\]

then the Lagrangian \( L(v, \mu) \) can be written as

\[
L(v, \mu) = J(v) + \sum_{i=1}^{m} \mu_i \varphi_i(v) = J(v) + \langle C^T \mu, v \rangle - \langle \mu, d \rangle.
\]

Since

\[
L(u, \lambda) = \inf_{v \in \mathbb{R}^n} L(v, \lambda),
\]

by Theorem 21.11(4) we must have

\[
\nabla J_u + C^T \lambda = 0,
\]

and since

\[
G(\lambda) = L(u, \lambda) = \sup_{\mu \in \mathbb{R}_+^m} L(u, \mu),
\]

by Theorem 21.11(3) (and since maximizing a function \( g \) is equivalent to minimizing \(-g\)), we must have

\[
G'_\lambda(\mu - \lambda) \leq 0 \quad \text{for all } \mu \in \mathbb{R}_+^m,
\]

and since \( \nabla G_\lambda = \varphi(u) \), we get

\[
\langle \varphi(u), \mu - \lambda \rangle \leq 0 \quad \text{for all } \mu \in \mathbb{R}_+^m.
\]

As in the proof of Proposition 30.14, \((**)_2\) can be expressed as follows for every \( \rho > 0 \):

\[
\langle \lambda - (\lambda + \rho \varphi(u)), \mu - \lambda \rangle \geq 0 \quad \text{for all } \mu \in \mathbb{R}_+^m,
\]

which shows that \( \lambda \) can be viewed as the projection onto \( \mathbb{R}_+^m \) of the vector \( \lambda + \rho \varphi(u) \). In summary we obtain the equations

\[
\left(\dagger_1\right) \quad \begin{cases} 
\nabla J_u + C^T \lambda = 0 \\
\lambda = p_+ (\lambda + \rho \varphi(u)).
\end{cases}
\]
CHAPTER 14. INTRODUCTION TO NONLINEAR OPTIMIZATION

Step 2. We establish algebraic conditions relating the unique solution $u_k$ of the minimization problem arising during an iteration of Uzawa’s method in (UZ) and $\lambda^k$.

Observe that the Lagrangian $L(v, \mu)$ is strictly convex as a function of $v$ (as the sum of a strictly convex function and an affine function). As in the proof of Theorem 30.7, we have

\[ J(v) + \langle C^T \mu, v \rangle \geq J(0) + \langle \nabla J_0, v \rangle + \frac{\alpha}{2} \| v \|^2 + \langle C^T \mu, v \rangle \]

\[ \geq J(0) - \| \nabla J_0 \| \| v \| - \| C^T \mu \| \| v \| + \frac{\alpha}{2} \| v \|^2 , \]

and the term $(-\| \nabla J_0 \| - \| C^T \mu \| \| v \| + \frac{\alpha}{2} \| v \|) \| v \|$ goes to $+\infty$ when $\| v \|$ tends to $+\infty$, so $L(v, \mu)$ is coercive as a function of $v$. Therefore, the minimization problem find $u^k$ such that

\[ J(u^k) + \sum_{i=1}^{m} \lambda^k_i \varphi_i(u^k) = \inf_{v \in \mathbb{R}^n} \left( J(v) + \sum_{i=1}^{m} \lambda^k_i \varphi_i(v) \right) \]

has a unique solution $u^k \in \mathbb{R}^n$. It follows from Theorem 21.11(4) that the vector $u^k$ must satisfy the equation

\[ \nabla J_{u^k} + C^T \lambda^k = 0, \tag{*3} \]

and since by definition of Uzawa’s method

\[ \lambda^{k+1} = p_+(\lambda^k + \rho \varphi(u^k)), \tag{*4} \]

we obtain the equations

\[ \begin{cases} \nabla J_{u^k} + C^T \lambda^k = 0 \\ \lambda^{k+1} = p_+(\lambda^k + \rho \varphi(u^k)). \end{cases} \tag{†2} \]

Step 3. By subtracting the first of the two equations of (†1) and (†2) we obtain

\[ \nabla J_{u^k} - \nabla J_u + C^T (\lambda^k - \lambda) = 0, \]

and by subtracting the second of the two equations of (†1) and (†2) and using Proposition 29.6, we obtain

\[ \| \lambda^{k+1} - \lambda \| \leq \| \lambda^k - \lambda + \rho C(u^k - u) \|. \]

In summary, we proved

\[ \begin{cases} \nabla J_{u^k} - \nabla J_u + C^T (\lambda^k - \lambda) = 0 \\ \| \lambda^{k+1} - \lambda \| \leq \| \lambda^k - \lambda + \rho C(u^k - u) \|. \end{cases} \tag{†} \]

Step 4. Convergence of the sequence $(u^k)_{k \geq 0}$ to $u$.

Squaring both sides of the inequality in (†) we obtain

\[ \| \lambda^{k+1} - \lambda \|^2 \leq \| \lambda^k - \lambda \|^2 + 2 \rho \langle C^T(u^k - u), u_k - u \rangle + \rho^2 \| u^k - u \|^2. \]
Using the equation in (†) and the inequality
\[
\langle \nabla J_{u^k} - \nabla J_u, u^k - u \rangle \geq \alpha \| u^k - u \|^2,
\]
we get
\[
\| \lambda^{k+1} - \lambda \|^2 \leq \| \lambda^k - \lambda \|^2 - 2\rho \langle \nabla J_{u^k} - \nabla J_u, u^k - u \rangle + \rho^2 \| u^k - u \|^2
\]
\[
\leq \| \lambda^k - \lambda \|^2 - \rho(2\alpha - \rho \| C \|^2_2) \| u^k - u \|^2.
\]
Consequently, if
\[
0 \leq \rho \leq \frac{2\alpha}{\| C \|^2_2},
\]
we have
\[
\| \lambda^{k+1} - \lambda \| \leq \| \lambda^k - \lambda \|, \quad \text{for all } k \geq 0.
\]
By (*5), the sequence \((\| \lambda^k - \lambda \|)_{k \geq 0}\) is nonincreasing and bounded below by 0, so it converges, which implies that
\[
\lim_{k \to \infty} \left( \| \lambda^{k+1} - \lambda \| - \| \lambda^k - \lambda \| \right) = 0,
\]
and since
\[
\| \lambda^{k+1} - \lambda \|^2 \leq \| \lambda^k - \lambda \|^2 - \rho(2\alpha - \rho \| C \|^2_2) \| u^k - u \|^2,
\]
we also have
\[
\rho(2\alpha - \rho \| C \|^2_2) \| u^k - u \|^2 \leq \| \lambda^k - \lambda \|^2 - \| \lambda^{k+1} - \lambda \|^2,
\]
so if
\[
0 < \rho < \frac{2\alpha}{\| C \|^2_2},
\]
then \(\rho(2\alpha - \rho \| C \|^2_2) > 0\), and we conclude that
\[
\lim_{k \to \infty} \| u^k - u \| = 0,
\]
that is, the sequence \((u^k)_{k \geq 0}\) converges to \(u\).

**Step 5.** Convergence of the sequence \((\lambda^k)_{k \geq 0}\) to \(\lambda\) if \(C\) has rank \(m\).

Since the sequence \((\| \lambda^k - \lambda \|)_{k \geq 0}\) is nonincreasing the sequence \((\lambda^k)_{k \geq 0}\) is bounded, and thus it has a convergent subsequence \((\lambda^{i(k)})_{i \geq 0}\) whose limit is some \(\lambda' \in \mathbb{R}^m\). Since \(J'\) is continuous, by (†) we have
\[
\nabla J_u + C^T \lambda' = \lim_{i \to \infty} (\nabla J_{u^{(i)}} + C^T \lambda^{i(k)}) = 0.
\]
\[(*)_6\]

If \(C\) has rank \(m\), then \(\text{Im}(C) = \mathbb{R}^m\), which is equivalent to \(\text{Ker}(C^T) = (0)\), so \(C^T\) is injective and since by (†1) we also have \(\nabla J_u + C^T \lambda = 0\), we conclude that \(\lambda' = \lambda\). The above reasoning applies to any subsequence of \((\lambda^k)_{k \geq 0}\), so \((\lambda^k)_{k \geq 0}\) converges to \(\lambda\). \(\square\)
In the special case where $J$ is an elliptic quadratic functional

$$J(v) = \frac{1}{2} \langle Av, v \rangle - \langle b, v \rangle,$$

where $A$ is symmetric positive definite, an iteration of Uzawa’s method gives

$$Au^k - b + C^T \lambda^k = 0$$
$$\lambda^{k+1}_i = \max \{ (\lambda^k + \rho(Cu^k - d))_i, 0 \}, \quad 1 \leq i \leq m.$$

Theorem 31.18 implies that Uzawa’s method converges if

$$0 < \rho < \frac{2\lambda_1}{\|C\|_2^2},$$

where $\lambda_1$ is the smallest eigenvalue of $A$.

If we solve for $u^k$ using the first equation, we get

$$\lambda^{k+1} = p_+ (\lambda^k + \rho (-CA^{-1}C^T \lambda^k + CA^{-1}b - d)). \quad (\ast_7)$$

In Example 31.7 we showed that the gradient of the dual function $G$ is given by

$$\nabla G_\mu = Cu_\mu - d = -CA^{-1}C^T \mu + CA^{-1}b - d,$$

so $(\ast_7)$ can be written as

$$\lambda^{k+1} = p_+ (\lambda^k + \rho \nabla \lambda^k);$$

this shows that Uzawa’s method is indeed the gradient method with fixed stepsize applied to the dual program.

### 14.10 Summary

The main concepts and results of this chapter are listed below:

- The cone of feasible directions.
- Cone with apex.
- Active and inactive constraints.
- Qualified constraint at $u$.
- Farkas lemma.
- Farkas–Minkowski lemma.
- Karush–Kuhn–Tucker optimality conditions (or $KKT$-conditions).
• Complementary slackness conditions.
• Generalized Lagrange multipliers.
• Qualified convex constraint.
• Lagrangian of a minimization problem.
• Hard margin support vector machine
• Training data
• Linearly separable sets of points.
• Maximal margin hyperplane.
• Support vectors
• Lagrangian duality.
• Saddle points.
• Lagrange dual function.
• Lagrange dual program.
• Duality gap.
• Weak duality.
• Strong Duality.
• Handling equality constraints in the Lagrangian.
• Dual of the Hard margin SVM (SVM$_{h2}$).
• Conjugate functions and Legendre dual functions.
• Dual of the Hard margin SVM (SVM$_{h1}$).
Part IV

Applications to Machine Learning
Chapter 15

Ridge Regression and Lasso Regression

15.1 Ridge Regression

The problem of solving an overdetermined or underdetermined linear system $Ax = y$ arises as a “learning problem” in which we observe a sequence of data $((a_1, y_1), \ldots, (a_m, y_m))$, where $a_i \in \mathbb{R}^n$ and $y_i \in \mathbb{R}$, viewed as input-output pairs of some unknown function $f$ that we are trying to infer. The simplest kind of function is a linear function $f(x) = x^\top w$, where $w \in \mathbb{R}^n$ is a vector of coefficients usually called a weight vector. Since the problem is overdetermined and since our observations may be subject to errors, we can’t solve for $w$ exactly as the solution of the system $Aw = y$, so instead we solve the least-square problem of minimizing $\|Aw - y\|^2$.

In Section 17.1 (Vol. I) we showed that this problem can be solved using the pseudo-inverse. We know that the minimizers $w$ are solutions of the normal equations $A^\top Aw = A^\top y$, but when $A^\top A$ is not invertible, such a solution is not unique so some criterion has to be used to choose among these solutions.

The pseudo-inverse does so in a specific way that sets some of the components to 0. This is not always desirable and another way is to control the size of $w$ by adding a regularization term to $\|Aw - y\|^2$, and a natural candidate is $\|w\|^2$. It is also customary to view each row of the matrix $A$ as the transpose of an input vector $x_i \in \mathbb{R}^n$, and to define the $m \times n$ matrix $X$ as

$$X = \begin{pmatrix} x_1^\top \\ \vdots \\ x_m^\top \end{pmatrix},$$

where the row vectors $x_i^\top$ are the rows of $X$, and thus the $x_i \in \mathbb{R}^n$ are column vectors. Our optimization problem, called ridge regression, is the problem (RR1):

$$\text{minimize} \quad \|y - Xw\|^2 + K \|w\|^2,$$
which by introducing the new variable $\xi = y - Xw$ can be rewritten as (RR2):

$$\begin{align*}
\text{minimize} & \quad \xi^\top \xi + Kw^\top w \\
\text{subject to} & \quad y - Xw = \xi,
\end{align*}$$

where $K > 0$ is some constant determining the influence of the regularizing term $w^\top w$.

The objective function of the first version of our minimization problem can be expressed as

$$J(w) = \|y - Xw\|^2 + K\|w\|^2 = (y - Xw)^\top(y - Xw) + Kw^\top w = y^\top y - 2w^\top X^\top y + w^\top X^\top Xw + Kw^\top w = w^\top (X^\top X + KI_n)w - 2w^\top X^\top y + y^\top y.$$ 

The matrix $X^\top X$ is symmetric positive semidefinite and $K > 0$, so the matrix $X^\top X + KI_n$ is positive definite. It follows that $J(w)$ is strictly convex, so it has a unique minimum iff $\nabla J_w = 0$. Since $\nabla J_w = 2(X^\top X + KI_n)w - 2X^\top y,$

we deduce that

$$w = (X^\top X + KI_n)^{-1}X^\top y.$$  \hfill (\ast_{wp})$$

The dual function of the first formulation of our problem is a constant function (with value the minimum of $J$) so it is not useful, but the second formulation of our problem yields an interesting dual problem. The Lagrangian is

$$L(\xi, w, \lambda) = \xi^\top \xi + Kw^\top w + (y - Xw - \xi)^\top \lambda = \xi^\top \xi + Kw^\top w - w^\top X^\top \lambda - \xi^\top \lambda + \lambda^\top y.$$ 

with $\lambda, \xi, y \in \mathbb{R}^m$.

To derive the dual function $G(\lambda)$ we minimize $L(\xi, w, \lambda)$ with respect to $\xi$ and $w$, and for this we set the gradient $\nabla L_{\xi,w}$ to zero. Since

$$\nabla L_{\xi,w} = \begin{pmatrix} 2\xi - \lambda \\ 2Kw - X^\top \lambda \end{pmatrix},$$

we get

$$\lambda = 2\xi$$

$$w = \frac{1}{2K}X^\top \lambda = X^\top \frac{\xi}{K}.$$
15.1. RIDGE REGRESSION

The above suggests defining the variable $\alpha$ so that $\xi = K\alpha$, so we have $\lambda = 2K\alpha$ and $w = X^T\alpha$. Then we obtain the dual function as a function of $\alpha$ by substituting the above values of $\xi, \lambda$ and $w$ back in the Lagrangian and we get

$$G(\alpha) = K^2\alpha^T\alpha + K\alpha^TXX^T\alpha - 2K\alpha^TXX^T\alpha - 2K^2\alpha^T\alpha + 2K\alpha^Ty$$

$$= -K\alpha^T(XX^T + KI_m)\alpha + 2K\alpha^Ty.$$

This is a strictly concave function so its maximum is achieved iff $\nabla G_\alpha = 0$, that is,

$$2K(XX^T + KI_m)\alpha = 2Ky,$$

which yields

$$\alpha = (XX^T + KI_m)^{-1}y.$$

Putting everything together we obtain

$$\alpha = (XX^T + KI_m)^{-1}y$$

$$w = X^T\alpha$$

$$\xi = K\alpha,$$

which yields

$$w = X^T(XX^T + KI_m)^{-1}y. \quad \text{(*)}_{wd}$$

Earlier in (\text{*}_{wp}) we found that

$$w = (X^TX + KI_n)^{-1}X^Ty,$$

and it is easy to check that

$$(X^TX + KI_n)^{-1}X^T = X^T(XX^T + KI_m)^{-1}.$$

It is easy to adapt the above method to learn an affine function $f(w) = x^Tw + b$ instead of a linear function $f(w) = x^Tw$, where $b \in \mathbb{R}$. We have the following optimization program (RR3):

$$\text{minimize} \quad \xi^T\xi + Kw^Tw$$

subject to

$$y - Xw - b1 = \xi,$$

with $y, \xi, 1 \in \mathbb{R}^m$ and $w \in \mathbb{R}^n$. Note that in program (RR3), minimization is only performed over $\xi$ and $w$, but not over the variable $b$. The Lagrangian associated with this program is

$$L(\xi, w, b, \lambda) = \xi^T\xi + Kw^Tw - w^TXX^T\lambda - \xi^T\lambda - b1^T\lambda + \lambda^Ty.$$
By setting the gradient $\nabla L_{\xi,b,w}$ to zero, we get

$$
\begin{align*}
\lambda &= 2\xi \\
1^T\lambda &= 0 \\
w &= \frac{1}{2K}X^T\lambda = X^T\frac{\xi}{K}.
\end{align*}
$$

As before, if we set $\xi = K\alpha$, we obtain $w = X^T\alpha$ and

$$
G(\alpha) = -K\alpha^T(XX^T + KI_m)\alpha + 2K\alpha^Ty.
$$

Since $K > 0$ and $\lambda = 2K\alpha$, the dual to ridge regression is the following program ($\text{DRR3}$):

$$
\begin{align*}
\text{minimize} & \quad \alpha^T(XX^T + KI_m)\alpha - 2\alpha^Ty \\
\text{subject to} & \quad 1^T\alpha = 0.
\end{align*}
$$

Observe that up to the factor $1/2$, this problem satisfies the conditions of Proposition 23.3 with $A = (XX^T + KI_m)^{-1}$, $b = y$, $B = 1_m$, $f = 0$, and $x$ renamed as $\alpha$. Therefore, it has a unique solution $\alpha$ (beware that $\lambda = 2K\alpha$ is not the $\lambda$ used in Proposition 23.3, which we rename as $\mu$). Since the solution given by Proposition 23.3 is

$$
\mu = (B^T AB)^{-1}(B^T Ab - f), \quad \alpha = A(b - B\mu),
$$

we get

$$
\mu = (1^T (XX^T + KI_m)^{-1} 1)^{-1} 1^T (XX^T + KI_m)^{-1} y, \quad \alpha = (XX^T + KI_m)^{-1} (y - \mu 1).
$$

Note that the matrix $B^T AB$ is the scalar $1^T (XX^T + KI_m)^{-1} 1$.

Once $\alpha, \xi = K\alpha$, and $w = X^T\alpha$ are determined, $b$ is given by the equation

$$
b = y - Xw - \xi = y - Xw - K\alpha.
$$

Since $1^T1 = m$ and $1^T\alpha = 0$, we get

$$
b = \frac{1}{m}1^Ty - \frac{1}{m}1^TXw - \frac{1}{m}K1^T\alpha = \bar{y} - \sum_{j=1}^{n} \overline{X^j}w_j,
$$

where $\bar{y}$ is the mean of $y$ and $\overline{X^j}$ is the mean of the $j$th column of $X$. Therefore,

$$
b = \bar{y} - \sum_{j=1}^{n} \overline{X^j}w_j = \bar{y} - (X^T \cdots \overline{X^n})w,
$$
where \((\overline{X^1} \cdots \overline{X^n})\) is the \(1 \times n\) row vector whose \(j\)th entry is \(\overline{X^j}\). Since \(w = X^\top \alpha\), we can also write
\[
b = \overline{y} - \frac{1}{m} \mathbf{1}^\top XX^\top \alpha.
\]

The expression
\[
b = \overline{y} - (\overline{X^1} \cdots \overline{X^n})w
\]
suggests looking for an intercept term \(b\) (also called bias) of the above form, namely the program \((\text{RR4})\):
\[
\begin{align*}
\text{minimize} & \quad \xi^\top \xi + Kw^\top w \\
\text{subject to} & \quad y - Xw - b1 = \xi \\
& \quad b = \hat{b} + \overline{y} - (\overline{X^1} \cdots \overline{X^n})w,
\end{align*}
\]
with \(\hat{b} \in \mathbb{R}\). Again, in program \((\text{RR4})\), minimization is only performed over \(\xi\) and \(w\). Since
\[
b1 = \hat{b}1 + \overline{y}1 - (\overline{X^1} \cdots \overline{X^n}1)w,
\]
if \(\overline{X} = (\overline{X^1} \cdots \overline{X^n})\) is the \(m \times n\) matrix whose \(j\)th column is the vector \(\overline{X^j}\), then the above program is equivalent to the program \((\text{RR5})\):
\[
\begin{align*}
\text{minimize} & \quad \xi^\top \xi + Kw^\top w \\
\text{subject to} & \quad \hat{y} - \hat{X}w - \hat{b}1 = \xi,
\end{align*}
\]
If we write \(\hat{y} = y - \overline{y}1\) and \(\hat{X} = X - \overline{X}\), then the above program becomes \((\text{RR6})\):
\[
\begin{align*}
\text{minimize} & \quad \xi^\top \xi + Kw^\top w \\
\text{subject to} & \quad \hat{y} - \hat{X}w - \hat{b}1 = \xi.
\end{align*}
\]
If the solution to this program is \(\hat{w}\), then \(\hat{b}\) is given by
\[
\hat{b} = \overline{y} - (\overline{X^1} \cdots \overline{X^n})\hat{w} = 0,
\]
since the data \(\hat{y}\) and \(\hat{X}\) are centered. Therefore \((\text{RR6})\) is equivalent to ridge regression without an intercept term applied to the centered data \(\hat{y} = y - \overline{y}1\) and \(\hat{X} = X - \overline{X}\), program \((\text{RR6'})\):
\[
\begin{align*}
\text{minimize} & \quad \xi^\top \xi + Kw^\top w \\
\text{subject to} & \quad \hat{y} - \hat{X}w = \xi.
\end{align*}
\]
If \( \hat{w} \) is the optimal solution of this program given by
\[
\hat{w} = \hat{X}^\top (\hat{X} \hat{X}^\top + K I_m)^{-1} \hat{y},
\]
then \( b \) is given by
\[
b = \bar{y} - (\bar{X}^\top \cdots \bar{X}^n) \hat{w}.
\]

**Remark:** Although this is not obvious a priori, the optimal solution \( w^* \) of the program (RR3) is equal to the optimal solution \( \hat{w} \) of program (RR6'). However, in practice, since solving the dual (DRR3) is harder than solving the program (RR6'), because the dual program has the extra constraint \( 1^\top \alpha = 0 \), the program (RR6') involving the centered data is the preferred one.

It is natural to wonder what happens if we also minimize with respect to \( b \) in program (RR3). Let us add the term \( K b^2 \) to the objective function. Then we obtain the program
\[
\begin{align*}
\text{minimize} & \quad \xi^\top \xi + K w^\top w + K b^2 \\
\text{subject to} & \quad y - X w - b 1 = \xi.
\end{align*}
\]
This suggests treating \( b \) an an extra component of the weight vector \( w \) and by forming the \( m \times (n+1) \) matrix \([X \ 1]\) obtained by adding a column of 1's (of dimension \( m \)) to the matrix \( X \), we obtain the program (RR3b):
\[
\begin{align*}
\text{minimize} & \quad \xi^\top \xi + K w^\top w + K b^2 \\
\text{subject to} & \quad y - [X \ 1] \begin{pmatrix} w \\ b \end{pmatrix} = \xi.
\end{align*}
\]
This program is solved just as program (RR2) and, we get
\[
\begin{align*}
\alpha &= ([X \ 1][X \ 1]^\top + K I_m)^{-1} y \\
\begin{pmatrix} w \\ b \end{pmatrix} &= [X \ 1]^\top \alpha \\
\xi &= K \alpha.
\end{align*}
\]
Thus
\[
b = 1^\top \alpha.
\]
Observe that \([X \ 1][X \ 1]^\top = XX^\top + 11^\top \). Since we also have the equation
\[
y - X w - b 1 = \xi,
\]
we obtain
\[
\frac{1}{m} 1^\top y - \frac{1}{m} 1^\top X w - \frac{1}{m} b 1^\top 1 = \frac{1}{m} 1^\top K \alpha,
\]
so

\[ \mathbf{y} - (X^T \cdots X^n) \hat{w} - b = \frac{1}{m} K b, \]

which yields

\[ b = \frac{m}{m + K} (\mathbf{y} - (X^T \cdots X^n) w). \]

The exact same derivation holds with \( K \) replaced by an arbitrary constant \( C > 0 \), and we obtain

\[ b = \frac{m}{m + C} (\mathbf{y} - (X^T \cdots X^n) w). \]

As pointed out by Hastie, Tibshirani, and Friedman [53] (Section 3.4), a defect of the approach where \( b \) is also penalized is that the solution for \( b \) is not invariant under adding a constant \( c \) to each value \( y_i \). This is not the case for the approach using program (RR6').

One interesting aspect of the dual (of either (RR2) or (RR3)) is that it shows that the solution \( w \) being of the form \( X^T \alpha \), is a linear combination

\[ w = \sum_{i=1}^{m} \alpha_i x_i \]

of the data points \( x_i \), with the coefficients \( \alpha_i \) corresponding to the dual variable \( \lambda = 2K\alpha \) of the dual function, and with

\[ \alpha = (XX^T + KI_m)^{-1} y. \]

If \( m \) is smaller than \( n \), then it is more advantageous to solve for \( \alpha \). But what really makes the dual interesting is that with our definition of \( X \) as

\[ X = \begin{pmatrix} x_1^T \\ \vdots \\ x_m^T \end{pmatrix}, \]

the matrix \( XX^T \) consists of the inner products \( x_i^T x_j \), and similarly the function learned \( f(x) = w^T x \) can be expressed as

\[ f(x) = \sum_{i=1}^{m} \alpha_i x_i^T x, \]

namely that both \( w \) and \( f(x) \) are given in terms of the inner products \( x_i^T x_j \) and \( x_i^T x \).

This fact is the key to a generalization to ridge regression in which the input space \( \mathbb{R}^n \) is embedded in a larger (possibly infinite dimensional) Euclidean space \( F \) (with an inner product \( \langle -, - \rangle \)) usually called a feature space, using a function

\[ \varphi: \mathbb{R}^n \to F. \]
The problem becomes (kernel ridge regression) (KRR2):

\[
\begin{align*}
\text{minimize} \quad & \xi^\top \xi + K \langle w, w \rangle \\
\text{subject to} \quad & y_i - \langle w, \varphi(x_i) \rangle = \xi_i, \quad i = 1, \ldots, m.
\end{align*}
\]

Note that \( w \in F \). This problem is discussed in Shawe–Taylor and Christianini [97] (Section 7.3).

We will show below that the solution is exactly the same:

\[
\begin{align*}
\alpha &= (G + KI_m)^{-1} y \\
w &= \sum_{i=1}^m \alpha_i \varphi(x_i) \\
\xi &= K \alpha,
\end{align*}
\]

where \( G \) is the Gram matrix given by \( G_{ij} = \langle \varphi(x_i), \varphi(x_j) \rangle \). This matrix is also called the kernel matrix and is often denoted by \( K \) instead of \( G \).

In this framework, we have to be a little careful in using gradients since the inner product \( \langle -, - \rangle \) on \( F \) is involved and \( F \) could be infinite dimensional, but this causes no problem because we can use derivatives, and by Proposition 20.5 we have

\[
d\langle -, -, (u,v) \rangle (x,y) = \langle x, v \rangle + \langle u, y \rangle.
\]

This implies that the derivative of the map \( u \mapsto \langle u, u \rangle \) is

\[
d\langle -, -, u \rangle (x) = 2\langle x, u \rangle.
\]

Since the map \( u \mapsto \langle u, v \rangle \) (with \( v \) fixed) is linear, its derivative is

\[
d\langle -, v \rangle_u (x) = \langle x, v \rangle.
\]

The derivative of the Lagrangian

\[
L(\xi, w, \lambda) = \xi^\top \xi + K \langle w, w \rangle - \sum_{i=1}^m \lambda_i \langle \varphi(x_i), w \rangle - \xi^\top \lambda + \lambda^\top y
\]

with respect to \( \xi \) and \( w \) is

\[
dL_{\xi,w}(\widetilde{\xi}, \widetilde{w}) = 2(\widetilde{\xi})^\top \xi - (\widetilde{\xi})^\top \lambda + \left(2Kw - \sum_{i=1}^m \lambda_i \varphi(x_i), \widetilde{w}\right).
\]

We have \( dL_{\xi,w}(\widetilde{\xi}, \widetilde{w}) = 0 \) for all \( \widetilde{\xi} \) and \( \widetilde{w} \) iff

\[
2Kw = \sum_{i=1}^m \lambda_i \varphi(x_i)
\]

\[
\lambda = 2\xi.
\]
Again we define $\xi = K\alpha$, so we have $\lambda = 2K\alpha$, and

$$w = \sum_{i=1}^{m} \alpha_i \varphi(x_i).$$

Plugging back into the Lagrangian we get

$$G(\alpha) = K^2\alpha^\top\alpha + K \sum_{i,j=1}^{m} \alpha_i \alpha_j \langle \varphi(x_i), \varphi(x_j) \rangle - 2K \sum_{i,j=1}^{m} \alpha_i \alpha_j \langle \varphi(x_i), \varphi(x_j) \rangle$$

$$- 2K^2\alpha^\top\alpha + 2K\alpha^\top y$$

$$= -K^2\alpha^\top\alpha - K \sum_{i,j=1}^{m} \alpha_i \alpha_j \langle \varphi(x_i), \varphi(x_j) \rangle + 2K\alpha^\top y.$$ 

If $G$ is the matrix given by $G_{ij} = \langle \varphi(x_i), \varphi(x_j) \rangle$, then we have

$$G(\alpha) = -K\alpha^\top (G + KI_m)\alpha + 2K\alpha^\top y.$$ 

The function $G$ is strictly concave and has a maximum for

$$\alpha = (G + KI_m)^{-1} y,$$

as claimed earlier.

As in the standard case of ridge regression, if $F = \mathbb{R}^n$ (but the inner product $\langle -, - \rangle$ is arbitrary), we can adapt the above method to learn an affine function $f(w) = x^\top w + b$ instead of a linear function $f(w) = x^\top w$, where $b \in \mathbb{R}$. This time we assume that $b$ is of the form

$$b = \bar{y} - \langle w, (\overline{X^1} \cdots \overline{X^n}) \rangle,$$

where $X^j$ is the $j$ column of the $m \times n$ matrix $X$ whose $i$th row is the transpose of the column vector $\varphi(x_i)$, and where $(\overline{X^1} \cdots \overline{X^n})$ is viewed as a column vector. We have the minimization problem ($\text{KRR6}'$):

$$\text{minimize} \quad \xi^\top \xi + K\langle w, w \rangle$$

subject to

$$\widehat{y}_i - \langle w, \overline{\varphi(x_i)} \rangle = \xi_i, \quad i = 1, \ldots, m,$$

where $\overline{\varphi(x_i)}$ is the $n$-dimensional vector $\varphi(x_i) - (\overline{X^1} \cdots \overline{X^n})$.

The solution is given in terms of the matrix $\hat{G}$ defined by

$$\hat{G}_{ij} = \langle \overline{\varphi(x_i)}, \overline{\varphi(x_j)} \rangle,$$

as before. We get

$$\alpha = (\hat{G} + KI_m)^{-1} \hat{y},$$
and according to a previous computation, \( b \) is given by

\[
b = \bar{y} - \frac{1}{m} \mathbf{1} \hat{G} \alpha.
\]

We explain in Section 33.3 how to compute the matrix \( \hat{G} \) from the matrix \( G \).

Since the dimension of the feature space \( F \) may be very large, one might worry that computing the inner products \( \langle \varphi(x_i), \varphi(x_j) \rangle \) might be very expensive. This is where kernel functions come to the rescue. A kernel function \( \kappa \) for an embedding \( \varphi: \mathbb{R}^n \rightarrow F \) is a map \( \kappa: \mathbb{R}^n \times \mathbb{R}^n \rightarrow \mathbb{R} \) with the property that

\[
\kappa(u, v) = \langle \varphi(u), \varphi(v) \rangle \quad \text{for all} \quad u, v \in \mathbb{R}^n.
\]

If \( \kappa(u, v) \) can be computed in a reasonably cheap way, and if \( \varphi(u) \) can be computed cheaply, then the inner products \( \langle \varphi(x_i), \varphi(x_j) \rangle \) (and \( \langle \varphi(x_i), \varphi(x) \rangle \)) can be computed cheaply. Fortunately there are good kernel functions. Two very good sources on kernel methods are Schölkopf and Smola [86] and Shawe-Taylor and Christianini [97]. We will investigate kernels in Chapter 33.

15.2 Lasso Regression (\( \ell_1 \)-Regularized Regression)

The main weakness of ridge regression is that the estimated weight vector \( w \) usually has many nonzero coefficients. As a consequence, ridge regression does not scale up well. In practice, we need methods capable of handling millions of parameters, or more. A way to encourage sparsity of the vector \( w \), which means that many coordinates of \( w \) are zero, is to replace the quadratic penalty function \( K w^\top w = K \|w\|_2^2 \) by the penalty function \( K \|w\|_1 \), with the 2-norm replaced by the 1-norm.

This method was first proposed by Tibshirani around 1996, under the name lasso, which stands for “least absolute selection and shrinkage operator.” This method is also known as \( \ell_1 \)-regularized regression, but this is not as cute as “lasso,” which is used predominantly.

Given a set of training data \( \{(x_1, y_1), \ldots, (x_m, y_m)\} \), with \( x_i \in \mathbb{R}^n \) and \( y_i \in \mathbb{R} \), if \( X \) is the \( m \times n \) matrix

\[
X = \begin{pmatrix}
    x_1^\top \\
    \vdots \\
    x_m^\top 
\end{pmatrix},
\]

in which the row vectors \( x_i^\top \) are the rows of \( X \), then lasso regression if the following optimization problem (lasso1):

\[
\text{minimize} \quad \frac{1}{2} \xi^\top \xi + K \|w\|_1 \\
\text{subject to} \quad y - Xw = \xi,
\]
15.2. LASSO REGRESSION ($\ell_1$-REGULARIZED REGRESSION)

where $K > 0$ is some constant determining the influence of the regularizing term $\|w\|_1$.

The difficulty with the regularizing term $\|w\|_1 = |w_1| + \cdots + |w_n|$ is that the map $w \mapsto \|w\|_1$ is not differentiable for all $w$. This difficulty can be overcome by using subgradients, but the dual of the above program can also be obtained in an elementary fashion by using a trick that we already used, which is that if $x \in \mathbb{R}$, then $|x| = \max\{x, -x\}$.

Using this trick, by introducing a vector $\epsilon \in \mathbb{R}^n$ of nonnegative variables, we can rewrite lasso minimization as follows:

**lasso regularization (lasso2):**

minimize $\frac{1}{2}\xi^\top \xi + K1^\top \epsilon$

subject to

$y - Xw = \xi$

$w \leq \epsilon$

$-w \leq \epsilon$

$\epsilon \geq 0$,

with $y, \xi \in \mathbb{R}^m$ and $w, \epsilon, 1 \in \mathbb{R}^n$.

The constraints $w \leq \epsilon$ and $-w \leq \epsilon$ are equivalent to $|w_i| \leq \epsilon_i$ for $i = 1, \ldots, n$, and for an optimal solution, we must have $|w_i| = \epsilon_i$, that is, $\|w\|_1 = \epsilon_1 + \cdots + \epsilon_n$.

The Lagrangian $L(\xi, w, \epsilon, \lambda, \alpha_+, \alpha_-, \beta)$ is given by

$L(\xi, w, \epsilon, \lambda, \alpha_+, \alpha_-, \beta) = \frac{1}{2}\xi^\top \xi + K1^\top \epsilon + \lambda^\top (y - Xw - \xi) + \alpha_+^\top (w - \epsilon) + \alpha_-^\top (-w - \epsilon) - \beta^\top \epsilon$

$= \frac{1}{2}\xi^\top \xi - \xi^\top \lambda + \lambda^\top y + \epsilon^\top (K1 - \alpha_+ - \alpha_- - \beta) + w^\top (\alpha_+ - \alpha_- - X^\top \lambda)$,

with $\lambda \in \mathbb{R}^m$ and $\alpha_+, \alpha_-, \beta \in \mathbb{R}_+^n$. Since the objective function is convex and the constraints are affine (and thus qualified), the Lagrangian $L$ has a minimum with respect to the primal variables, $\xi, w, \epsilon$ iff $\nabla L_{\xi, w, \epsilon} = 0$. Since the gradient $\nabla L_{\xi, w, \epsilon}$ is given by

$\nabla L_{\xi, w, \epsilon} = \begin{pmatrix} \frac{\xi - \lambda}{\alpha_+ - \alpha_- - X^\top \lambda} \\ \alpha_+ - \alpha_- - X^\top \lambda \\ K1 - \alpha_+ - \alpha_- - \beta \end{pmatrix}$,

we obtain the equations

$\xi = \lambda$

$\alpha_+ - \alpha_- = X^\top \lambda$

$\alpha_+ + \alpha_- = K1 - \beta$. 
Using these equations, the dual function $G(\lambda, \alpha_+, \alpha_-, \beta) = \min_{\xi, \omega, \epsilon} L$ is given by

\[
G(\lambda, \alpha_+, \alpha_-, \beta) = \frac{1}{2} \xi^\top \xi - \xi^\top \lambda + \lambda^\top y \\
= \frac{1}{2} \lambda^\top \lambda - \lambda^\top \lambda + \lambda^\top y \\
= -\frac{1}{2} \lambda^\top \lambda + \lambda^\top y \\
= -\frac{1}{2} (\|y - \lambda\|_2^2 - \|y\|_2^2).
\]

Since $\beta \geq 0$, the constraint $\alpha_+ + \alpha_- = K1 - \beta$ is equivalent to

\[\alpha_+ + \alpha_- \leq K1.\]

Since $\alpha_+, \alpha_- \geq 0$, for any $i \in \{1, \ldots, n\}$ the minimum of $(\alpha_+)_i - (\alpha_-)_i$ is $-K$, and the maximum is $K$. If we recall that for any $z \in \mathbb{R}^n$,

\[\|z\|_{\infty} = \max_{1 \leq i \leq n} |z_i|,\]

it follows that the constraints

\[
\alpha_+ + \alpha_- \leq K1 \\
X^\top \lambda = \alpha_+ - \alpha_-
\]

are equivalent to

\[\|X^\top \lambda\|_{\infty} \leq K.\]

The above is equivalent to the $2n$ constraints

\[-K \leq (X^\top \lambda)_i \leq K, \quad 1 \leq i \leq n.\]

Therefore, the dual lasso program is given by

maximize $-\frac{1}{2} (\|y - \lambda\|_2^2 - \|y\|_2^2)$

subject to

\[\|X^\top \lambda\|_{\infty} \leq K,\]

which (since $\|y\|_2^2$ is a constant term) is equivalent to (Dlasso2):

minimize $\|y - \lambda\|_2^2$

subject to

\[\|X^\top \lambda\|_{\infty} \leq K.\]
In view of the constraint \( y - Xw = \xi \) and the fact that for an optimal solution we must have \( \xi = \lambda \), the following condition must hold:

\[
\|X^\top (Xw - y)\|_\infty \leq K. \tag{*}
\]

Also observe that for an optimal solution, we have

\[
\frac{1}{2} \|y - Xw\|_2^2 + w^\top X^\top (y - Xw) = \frac{1}{2} \|y\|_2^2 - w^\top X^\top y + \frac{1}{2}w^\top X^\top Xw + w^\top X^\top y - w^\top X^\top Xw
\]

\[
= \frac{1}{2} \left( \|y\|_2^2 - \|Xw\|_2^2 \right)
\]

\[
= \frac{1}{2} \left( \|y\|_2^2 - \|y - \lambda\|_2^2 \right) = G(\lambda).
\]

Since the objective function is convex and the constraints are qualified, the duality gap is zero, so for optimal solutions of the primal and the dual, \( G(\lambda) = L(\xi, w, \epsilon) \), that is

\[
\frac{1}{2} \|y - Xw\|_2^2 + w^\top X^\top (y - Xw) = \frac{1}{2} \|y\|_2^2 + K \|w\|_1 = \frac{1}{2} \|y - Xw\|_2^2 + K \|w\|_1,
\]

which yields the equation

\[
w^\top X^\top (y - Xw) = K \|w\|_1. \tag{**}
\]

The above is the inner product of \( w \) and \( X^\top (y - Xw) \), so whenever \( w_i \neq 0 \), since \( \|w\|_1 = |w_1| + \cdots + |w_n| \), in view of \( * \), we must have \( (X^\top (y - Xw))_i = K\text{sgn}(w_i) \). If

\[
S = \{i \in \{1, \ldots, n\} \mid w_i \neq 0\},
\]

if \( X_S \) denotes the matrix consisting of the columns of \( X \) indexed by \( S \), and if \( w_S \) denotes the vector consisting of the nonzero components of \( w \), then we have

\[
X_S^\top (y - X_Sw_S) = K\text{sgn}(w_S).
\]

We also have

\[
\|X_S^\top (y - X_Sw_S)\|_\infty \leq K
\]

where \( \overline{S} \) is the complement of \( S \).

The first equation yields

\[
X_S^\top X_Sw_S = X_S^\top y - K\text{sgn}(w_S),
\]

so if \( X_S^\top X_S \) is invertible (which will be the case if the columns of \( X \) are linearly independent), we get

\[
w_S = (X_S^\top X_S)^{-1}(X_S^\top y - K\text{sgn}(w_S)).
\]

In theory, if we know the support of \( w \) and the signs of its components, then \( w_S \) is determined, but in practice, this is useless since the problem is to find the support and the sign of the solution.
One way to solve lasso regression is to use the dual program to find \( \lambda = \xi \), and then to use linear programming to find \( w \) by solving the linear program arising from the lasso primal by holding \( \xi \) constant. There are also a number of variations of gradient descent; see Hastie, Tibshirani, and Wainwright [54].

In the preceding discussion, we made the simplifying assumption that we were trying to learn a linear function \( f(x) = w^\top x \). To learn an affine function \( f(x) = w^\top x + b \), we solve the following optimization problem (lasso3):

\[
\begin{align*}
\text{minimize} & \quad \frac{1}{2} \xi^\top \xi + K 1_n^\top \epsilon \\
\text{subject to} & \quad y - Xw - b 1_m = \xi \\
& \quad w \leq \epsilon \\
& \quad -w \leq \epsilon \\
& \quad \epsilon \geq 0.
\end{align*}
\]

Observe that as in the case of ridge regression, we are not minimizing over \( b \).

The Lagrangian associated with this optimization problem is

\[
L(\xi, w, \epsilon, b, \lambda, \alpha_+, \alpha_-, \beta) = \frac{1}{2} \xi^\top \xi - \xi^\top \lambda + \lambda^\top y - b 1^\top \lambda + \epsilon^\top (K 1 - \alpha_+ - \alpha_- - \beta) + w^\top (\alpha_+ - \alpha_- - X^\top \lambda),
\]

so by setting the gradient \( \nabla L_{\xi, w, \epsilon, b} \) to zero we obtain the equations

\[
\begin{align*}
\xi &= \lambda \\
\alpha_+ - \alpha_- &= X^\top \lambda \\
\alpha_+ + \alpha_- &= K 1 - \beta \\
1^\top \lambda &= 0,
\end{align*}
\]

Using these equations, we find that the dual function is also given by

\[
G(\lambda, \alpha_+, \alpha_-, \beta) = -\frac{1}{2} \left(\|y - \lambda\|_2^2 - \|y\|_2^2\right),
\]

and the dual lasso program is given by

\[
\begin{align*}
\text{maximize} & \quad -\frac{1}{2} \left(\|y - \lambda\|_2^2 - \|y\|_2^2\right) \\
\text{subject to} & \quad \|X^\top \lambda\|_\infty \leq K \\
& \quad 1^\top \lambda = 0,
\end{align*}
\]
15.2. LASSO REGRESSION (\(\ell_1\)-REGULARIZED REGRESSION)

which is equivalent to (Dlasso3):

\[
\begin{align*}
\text{minimize} & \quad \|y - \lambda\|_2^2 \\
\text{subject to} & \quad \|X^T \lambda\|_\infty \leq K \\
& \quad 1^T \lambda = 0.
\end{align*}
\]

Once \(\lambda = \xi\) and \(w\) are determined, we obtain \(b\) using the equation

\[
b1 = y - Xw - \xi,
\]

and since \(1^T 1 = m\) and \(1^T \xi = 1^T \lambda = 0\), the above yields

\[
b = \frac{1}{m} 1^T y - \frac{1}{m} 1^T Xw - \frac{1}{m} 1^T \xi = \bar{y} - \sum_{j=1}^n \bar{X}^j w_j,
\]

where \(\bar{y}\) is the mean of \(y\) and \(\bar{X}^j\) is the mean of the \(j\)th column of \(X\). The equation

\[
b = \hat{b} + \bar{y} - \sum_{j=1}^n \bar{X}^j w_j = \hat{b} + \bar{y} - (\bar{X}^1 \cdots \bar{X}^n) \hat{w},
\]

can be used, as in ridge regression (see Section 32.1), to show that the program (lasso3) is equivalent to applying lasso regression (lasso2) without an intercept term to the centered data, by replacing \(y\) by \(\hat{y} = y - \bar{y} 1\) and \(X\) by \(\hat{X} = X - \bar{X}\). Then \(b\) is given by

\[
b = \bar{y} - (\bar{X}^1 \cdots \bar{X}^n) \hat{w},
\]

where \(\hat{w}\) is the solution given by (lasso2). This is the method described by Hastie, Tibshirani, and Wainwright [54] (Section 2.2).

Another way to find \(b\) is to add the term \((C/2)b^2\) to the objective function, for some positive constant \(C\) obtaining the program (lasso4). This time the Lagrangian is

\[
L(\xi, w, \epsilon, b, \lambda, \alpha_+, \alpha_-, \beta) = \frac{1}{2} \xi^T \xi - \xi^T \lambda + \lambda^T y + \frac{C}{2} b^2 - b 1^T \lambda \\
+ \epsilon^T (K 1 - \alpha_+ - \alpha_- - \beta) + w^T (\alpha_+ - \alpha_- - X^T \lambda),
\]

so by setting the gradient \(\nabla L_{\xi, w, \epsilon, b}\) to zero we obtain the equations

\[
\begin{align*}
\xi &= \lambda \\
\alpha_+ - \alpha_- &= X^T \lambda \\
\alpha_+ + \alpha_- &= K 1 - \beta \\
Cb &= 1^T \lambda.
\end{align*}
\]
Thus $b$ is also determined, and the dual lasso program is identical to the first lasso dual (\textbf{Dlasso2}), namely

$$
\begin{align*}
\text{minimize} & \quad \|y - \lambda\|_2^2 \\
\text{subject to} & \quad \|X^T\lambda\|_\infty \leq K.
\end{align*}
$$

Since the equations $\xi = \lambda$ and

$$
y - Xw - b1 = \xi
$$

hold, from $Cb = 1^T\lambda$ we get

$$
\frac{1}{m}1^T y - \frac{1}{m}1^T Xw - \frac{1}{m}1^T 1 = \frac{1}{m}1^T \lambda,
$$

that is

$$
\bar{y} - (\bar{X}^1 \cdots \bar{X}^n)w - b = \frac{C}{m}b,
$$

which yields

$$
b = \frac{m}{m+C}(\bar{y} - (\bar{X}^1 \cdots \bar{X}^n)w).
$$

As in the case of ridge regression, a defect of the approach where $b$ is also penalized is that the solution for $b$ is not invariant under adding a constant $c$ to each value $y_i$

## 15.3 Summary

The main concepts and results of this chapter are listed below:

- Ridge regression.
- Kernel ridge regression.
- Kernel functions.
- Lasso regression.
Chapter 16

Positive Definite Kernels

16.1 Basic Properties of Positive Definite Kernels

Let $X$ be a nonempty set. If the set $X$ represents a set of highly nonlinear data, it may be advantageous to map $X$ into a space $H$ of much higher dimension called the feature space, using a function $\varphi : X \to H$ called a feature map. This idea is that $\varphi$ “unwinds” the description of the objects in $X$, in an attempt to make it linear. The space $H$ is usually a vector space equipped with an inner product $\langle -, - \rangle$. If $H$ is infinite dimensional, then we assume that it is a Hilbert space.

Many algorithms to analyze or classify data make use of the inner products $\langle \varphi(x), \varphi(y) \rangle$, where $x, y \in X$. Thus it is natural to make the following definition.

**Definition 16.1.** Let $X$ be a nonempty set, let $H$ be a (complex) Hilbert space, and let $\varphi : X \to H$ be a function called a feature map. The function $\kappa : X \times X \to \mathbb{C}$ given by

$$\kappa(x, y) = \langle \varphi(x), \varphi(y) \rangle, \quad x, y \in X,$$

is called a kernel function.

**Remark:** A feature map is often called a feature embedding, but this terminology is a bit misleading because it suggests that such a map is injective, which is not necessarily the case. Unfortunately, this terminology is used by most people.

**Example 16.1.** Suppose we have two feature maps $\varphi_1 : X \to \mathbb{R}^{n_1}$ and $\varphi_2 : X \to \mathbb{R}^{n_2}$, and let $\kappa_1(x, y) = \langle \varphi_1(x), \varphi_1(y) \rangle$ and $\kappa_2(x, y) = \langle \varphi_2(x), \varphi_2(y) \rangle$ be the corresponding kernel functions (where $\langle -, - \rangle$ is the standard inner product on $\mathbb{R}^n$). Define the feature map $\varphi : X \to \mathbb{R}^{n_1+n_2}$ by

$$\varphi(x) = (\varphi_1(x), \varphi_2(x)),$$

an $(n_1 + n_2)$-tuple. We have

$$\langle \varphi(x), \varphi(y) \rangle = \langle (\varphi_1(x), \varphi_2(x)), (\varphi_1(y), \varphi_2(y)) \rangle = \langle \varphi_1(x), \varphi_1(y) \rangle + \langle \varphi_2(x), \varphi_2(y) \rangle$$

$$= \kappa_1(x, y) + \kappa_2(x, y),$$
which shows that the map \( \kappa \) given by

\[
\kappa(x, y) = \kappa_1(x, y) + \kappa_2(x, y)
\]

is the kernel function corresponding to the feature map \( \varphi: X \rightarrow \mathbb{R}^{n_1+n_2} \).

**Example 16.2.** Let \( X \) be a subset of \( \mathbb{R}^2 \), and let \( \varphi_1: X \rightarrow \mathbb{R}^3 \) be the map given by

\[
\varphi_1(x_1, x_2) = (x_1^2, x_2^2, \sqrt{2}x_1x_2).
\]

Observe that linear relations in the feature space \( H = \mathbb{R}^3 \) correspond to quadratic relations in the input space (of data). We have

\[
\langle \varphi_1(x), \varphi_1(y) \rangle = \langle (x_1^2, x_2^2, \sqrt{2}x_1x_2), (y_1^2, y_2^2, \sqrt{2}y_1y_2) \rangle
= x_1^2y_1^2 + x_2^2y_2^2 + 2x_1x_2y_1y_2
= (x_1y_1 + x_2y_2)^2 = \langle x, y \rangle^2,
\]

where \( \langle x, y \rangle \) is the usual inner product on \( \mathbb{R}^2 \). Hence the function

\[
\kappa(x, y) = \langle x, y \rangle^2
\]

is a kernel function associated with the feature space \( \mathbb{R}^3 \).

If we now consider the map \( \varphi_2: X \rightarrow \mathbb{R}^4 \) given by

\[
\varphi_2(x_1, x_2) = (x_1^2, x_2^2, x_1x_2, x_1x_2),
\]

we check immediately that

\[
\langle \varphi_2(x), \varphi_2(y) \rangle = \kappa(x, z) = \langle x, y \rangle^2,
\]

which shows that the same kernel can arise from different maps into different feature spaces.

**Example 16.3.** Example 33.2 can be generalized as follows. Suppose we have a feature map \( \varphi_1: X \rightarrow \mathbb{R}^n \) and let \( \kappa_1(x, y) = \langle \varphi_1(x), \varphi_1(y) \rangle \) be the corresponding kernel function (where \( \langle -, - \rangle \) is the standard inner product on \( \mathbb{R}^n \)). Define the feature map \( \varphi: X \rightarrow \mathbb{R}^n \times \mathbb{R}^n \) by its \( n^2 \) components

\[
\varphi(x)(i,j) = (\varphi_1(x))_i(\varphi_1(x))_j, \quad 1 \leq i, j \leq n,
\]

with the inner product on \( \mathbb{R}^n \times \mathbb{R}^n \) given by

\[
\langle u, v \rangle = \sum_{i,j=1}^n u(i,j)v(i,j).
\]
Then we have

\[
\langle \varphi(x), \varphi(y) \rangle = \sum_{i,j=1}^{n} \varphi_{(i,j)}(x)\varphi_{(i,j)}(y)
\]

\[
= \sum_{i,j=1}^{n} (\varphi_1(x))_i(\varphi_1(x))_j(\varphi_1(y))_i(\varphi_1(y))_j
\]

\[
= \sum_{i=1}^{n} (\varphi_1(x))_i(\varphi_1(y))_i \sum_{j=1}^{n} (\varphi_1(x))_j(\varphi_1(y))_j
\]

\[
= (\kappa_1(x,y))^2.
\]

Thus the map \( \kappa \) given by \( \kappa(x,y) = (\kappa_1(x,y))^2 \) is a kernel map associated with the feature map \( \varphi : X \to \mathbb{R}^n \times \mathbb{R}^n \). The feature map \( \varphi \) is a direct generalization of the feature map \( \varphi_2 \) of Example 33.2.

The above argument is immediately adapted to show that if \( \varphi_1 : X \to \mathbb{R}^{n_1} \) and \( \varphi_2 : X \to \mathbb{R}^{n_2} \) are two feature maps and if \( \kappa_1(x,y) = \langle \varphi_1(x), \varphi_1(y) \rangle \) and \( \kappa_2(x,y) = \langle \varphi_2(x), \varphi_2(y) \rangle \) are the corresponding kernel functions, then the map defined by

\[
\kappa(x,y) = \kappa_1(x,y)\kappa_2(x,y)
\]

is a kernel function, for the feature space \( \mathbb{R}^{n_1} \times \mathbb{R}^{n_2} \) and the feature map

\[
\varphi(x)_{(i,j)} = (\varphi_1(x))_i(\varphi_2(x))_j, \quad 1 \leq i \leq n_1, 1 \leq j \leq n_2.
\]

**Example 16.4.** Note that the feature map \( \varphi : X \to \mathbb{R}^n \times \mathbb{R}^n \) is not very economical because if \( i \neq j \) then the components \( \varphi_{(i,j)}(x) \) and \( \varphi_{(j,i)}(x) \) are both equal to \( (\varphi_1(x))_i(\varphi_1(x))_j \). Therefore we can define the more economical embedding \( \varphi' : X \to \mathbb{R}^{(n+1)/2} \) given by

\[
\varphi'(x)_{(i,j)} = \begin{cases} 
(\varphi_1(x))_i^2 & i = j, \\
\sqrt{2}(\varphi_1(x))_i(\varphi_1(x))_j & i < j,
\end{cases}
\]

where the pairs \((i, j)\) with \( 1 \leq i \leq j \leq n \) are ordered lexicographically. The feature map \( \varphi \) is a direct generalization of the feature map \( \varphi_1 \) of Example 33.2.

Observe that \( \varphi' \) can also be defined in the following way which makes it easier to come up with the generalization to any power:

\[
\varphi'_{(i_1, \ldots, i_n)}(x) = \left( \frac{2}{i_1 \cdots i_n} \right)^{1/2} (\varphi_1(x))_{i_1}^{i_1} (\varphi_1(x))_{i_2}^{i_2} \cdots (\varphi_1(x))_{i_n}^{i_n}, \quad i_1 + i_2 + \cdots + i_n = 2, i_j \in \mathbb{N},
\]

where the \( n \)-tuples \((i_1, \ldots, i_n)\) are ordered lexicographically. Recall that for any \( m \geq 1 \) and any \((i_1, \ldots, i_n) \in \mathbb{N}^m\) such that \( i_1 + i_2 + \cdots + i_n = m \), we have

\[
\binom{m}{i_1 \cdots i_n} = \frac{m!}{i_1! \cdots i_n!}.
\]
More generally, for any \( m \geq 2 \), using the multinomial theorem, we can define a feature embedding \( \varphi : X \to \mathbb{R}^{\binom{n+m-1}{m}} \) defining the kernel function \( \kappa \) given by \( \kappa(x, y) = (\kappa_1(x, y))^m \), with \( \varphi \) given by

\[
\varphi(i_1, \ldots, i_n)(x) = \left( \begin{array}{c} m \\ i_1 \cdots i_n \end{array} \right)^{1/2} (\varphi_1(x))^{i_1} (\varphi_1(x))^{i_2} \cdots (\varphi_1(x))^{i_n}, \quad i_1 + i_2 + \cdots + i_n = m, \quad i_j \in \mathbb{N},
\]

where the \( n \)-tuples \((i_1, \ldots, i_n)\) are ordered lexicographically.

**Example 16.5.** For any positive real constant \( R > 0 \), the constant function \( \kappa(x, y) = R \) is a kernel function corresponding to the feature map \( \varphi : X \to \mathbb{R} \) given by \( \varphi(x, y) = \sqrt{R} \).

By definition, the function \( \kappa'_1 : \mathbb{R}^n \to \mathbb{R} \) given by \( \kappa'_1(x, y) = \langle x, y \rangle \) is a kernel function (the feature map is the identity map from \( \mathbb{R}^n \) to itself). We just saw that for any positive real constant \( R > 0 \), the constant \( \kappa'_2(x, y) = R \) is a kernel function. By Example 33.1, the function \( \kappa'_3(x, y) = \kappa'_1(x, y) + \kappa'_2(x, y) \) is a kernel function, and for any integer \( d \geq 1 \), by Example 33.3, the function \( \kappa_d \) given by

\[
\kappa_d(x, y) = (\kappa'_3(x, y))^d = (\langle x, y \rangle + R)^d,
\]

is a kernel function on \( \mathbb{R}^n \). By the binomial formula,

\[
\kappa_d(x, y) = \sum_{m=0}^{d} \binom{d}{m} (\langle x, y \rangle)^m.
\]

By Example 33.1, the feature map of this kernel function is the concatenation of the features of the \( d+1 \) kernel maps \( R^{d-m}(x, y)^m \). By Example 33.3, the components of the feature map of the kernel map \( R^{d-m}(x, y)^m \) are reweightings of the functions

\[
\varphi(i_1, \ldots, i_n)(x) = x_1^{i_1} x_2^{i_2} \cdots x_n^{i_n}, \quad i_1 + i_2 + \cdots + i_n = m,
\]

with \((i_1, \ldots, i_n) \in \mathbb{N}^n\). Thus the components of the feature map of the kernel function \( \kappa_d \) are reweightings of the functions

\[
\varphi(i_1, \ldots, i_n)(x) = x_1^{i_1} x_2^{i_2} \cdots x_n^{i_n}, \quad i_1 + i_2 + \cdots + i_n \leq d,
\]

with \((i_1, \ldots, i_n) \in \mathbb{N}^n\). It is easy to see that the dimension of this feature space is \( \binom{m+d}{d} \).

There are a number of variations of the polynomial kernel \( \kappa_d \); all-subsets embedding kernels, ANOVA kernels; see Shawe–Taylor and Christianini [97], Chapter III.

In the next example, the set \( X \) is not a vector space.

**Example 16.6.** Let \( D \) be a finite set and let \( X = 2^D \) be its power set. If \(|D| = n\), let \( H = \mathbb{R}^X \cong \mathbb{R}^{2^n} \). We are assuming that the subsets of \( D \) are enumerated in some
fashion so that each coordinate of $\mathbb{R}^{2^n}$ corresponds to one of these subsets. For example, if $D = \{1, 2, 3, 4\}$, let

- $U_1 = \emptyset$
- $U_2 = \{1\}$
- $U_3 = \{2\}$
- $U_4 = \{3\}$
- $U_5 = \{4\}$
- $U_6 = \{1, 2\}$
- $U_7 = \{1, 3\}$
- $U_8 = \{1, 4\}$
- $U_9 = \{2, 3\}$
- $U_{10} = \{2, 4\}$
- $U_{11} = \{3, 4\}$
- $U_{12} = \{1, 2, 3\}$
- $U_{13} = \{1, 2, 4\}$
- $U_{14} = \{1, 3, 4\}$
- $U_{15} = \{2, 3, 4\}$
- $U_{16} = \{1, 2, 3, 4\}$

Let $\varphi : X \to H$ be the feature map defined as follows: for any subsets $A, U \in X$,

$$\varphi(A)_U = \begin{cases} 1 & \text{if } U \subseteq A \\ 0 & \text{otherwise.} \end{cases}$$

For example, if $A_1 = \{1, 2, 3\}$, we obtain the vector

$$\varphi(\{1, 2, 3\}) = (1, 1, 1, 1, 0, 1, 1, 0, 1, 0, 0, 0, 0, 0),$$

and if $A_2 = \{2, 3, 4\}$, we obtain the vector

$$\varphi(\{2, 3, 4\}) = (1, 0, 1, 1, 1, 0, 0, 0, 1, 1, 1, 0, 0, 0, 1, 0).$$

For any two subsets $A_1$ and $A_2$ of $D$, it is easy to check that

$$\langle \varphi(A_1), \varphi(A_2) \rangle = 2^{|A_1 \cap A_2|},$$

the number of common subsets of $A_1$ and $A_2$. For example, $A_1 \cap A_2 = \{2, 3\}$, and

$$\langle \varphi(A_1), \varphi(A_2) \rangle = 4.$$

Therefore, the function $\kappa : X \times X \to \mathbb{R}$ given by

$$\kappa(A_1, A_2) = 2^{|A_1 \cap A_2|}, \quad A_1, A_2 \subseteq D$$

is a kernel function.

Kernel functions have the following important property.

**Proposition 16.1.** Let $X$ be any nonempty set, let $H$ be any (complex) Hilbert space, let $\varphi : X \to H$ be any function, and let $\kappa : X \times X \to \mathbb{C}$ be the kernel given by

$$\kappa(x, y) = \langle \varphi(x), \varphi(y) \rangle, \quad x, y \in X.$$

For any finite subset $S = \{x_1, \ldots, x_p\}$ of $X$, if $K_S$ is the $p \times p$ matrix

$$K_S = (\kappa(x_j, x_i))_{1 \leq i, j \leq p} = (\langle \varphi(x_j), \varphi(x_i) \rangle)_{1 \leq i, j \leq p},$$

then we have

$$u^* K_S u \geq 0, \quad \text{for all } u \in \mathbb{C}^p.$$
Proof. We have

\[ u^*K_Su = u^\top K_S^\top u = \sum_{i,j=1}^{p} \kappa(x_i, x_j)u_i \overline{u_j} \]

\[ = \sum_{i,j=1}^{p} \langle \varphi(x), \varphi(y) \rangle u_i \overline{u_j} \]

\[ = \left\langle \sum_{i=1}^{p} u_i \varphi(x_i), \sum_{j=1}^{p} u_j \varphi(x_j) \right\rangle = \left\| \sum_{i=1}^{p} u_i \varphi(x_i) \right\|^2 \geq 0, \]

as claimed. \qed

Proposition 33.1 suggests a second approach to kernel functions which does not assume that a feature space and a feature map are provided. We will see in Section 33.2 that the two approaches are equivalent. The second approach is useful in practice because it is often difficult to define a feature space and a feature map in a simple manner.

Definition 16.2. Let \( X \) be a nonempty set. A function \( \kappa: X \times X \to \mathbb{C} \) is a positive definite kernel if for every finite subset \( S = \{x_1, \ldots, x_p\} \) of \( X \), if \( K_S \) is the \( p \times p \) matrix

\[ K_S = (\kappa(x_j, x_i))_{1 \leq i, j \leq p} \]

called a Gram matrix, then we have

\[ u^*K_Su = \sum_{i,j=1}^{p} \kappa(x_i, x_j)u_i \overline{u_j} \geq 0, \quad \text{for all } u \in \mathbb{C}^p. \]

Observe that Definition 33.2 does not require that \( u^*K_Su > 0 \) if \( u \neq 0 \), so the terminology positive definite is a bit abusive, and it would be more appropriate to use the terminology positive semidefinite. However, it seems customary to use the term positive definite kernel, or even positive kernel.

Proposition 16.2. Let \( \kappa: X \times X \to \mathbb{C} \) be a positive definite kernel. Then \( \kappa(x, x) \geq 0 \) for all \( x \in X \), and for any finite subset \( S = \{x_1, \ldots, x_p\} \) of \( X \), the \( p \times p \) matrix \( K_S \) given by

\[ K_S = (\kappa(x_j, x_i))_{1 \leq i, j \leq p} \]

is hermitian, that is, \( K_S^* = K_S \).

Proof. The first property is obvious by choosing \( S = \{x\} \). We have

\[ (u + v)^*K_S(u + v) = u^*K_Su + u^*K_Sv + v^*K_Su + v^*K_Sv, \]
and since \((u + v)^*K_S(u + v), u^*K_S u, v^*K_S v \geq 0\), we deduce that
\[
2A = u^*K_S v + v^*K_S u
\]
\[(1)\]
must be real. By replacing \(u\) by \(iu\), we see that
\[
2B = -iu^*K_s v + iv^*K_S u
\]
\[(2)\]
must also be real. By multiplying Equation (2) by \(i\) and adding it to Equation (1) we get
\[
u^*K_S v = A + iB.
\]
\[(3)\]
By subtracting Equation (3) from Equation (1) we get
\[
v^*K_S u = A - iB.
\]
Then
\[
u^*K_S^* v = v^*K_{SU} = A - iB = A + iB = u^*K_S v,
\]
for all \(u, v \in \mathbb{C}^*\), which implies \(K_S^* = K_S\). \(\Box\)

If the map \(\kappa: X \times X \rightarrow \mathbb{R}\) is real-valued, then we have the following criterion for \(\kappa\) to be a positive definite kernel that only involves real vectors.

**Proposition 16.3.** If \(\kappa: X \times X \rightarrow \mathbb{R}\), then \(\kappa\) is a positive definite kernel iff for any finite subset \(S = \{x_1, \ldots, x_p\}\) of \(X\), the \(p \times p\) real matrix \(K_S\) given by
\[
K_S = (\kappa(x_k, x_j))_{1 \leq j, k \leq p}
\]
is symmetric, that is, \(K_S^\top = K_S\), and
\[
u^\top K_S u = \sum_{j,k=1}^p \kappa(x_j, x_k)u_ju_k \geq 0, \quad \text{for all } u \in \mathbb{R}^p.
\]

**Proof.** If \(\kappa\) is a real-valued positive definite kernel, then the proposition is a trivial consequence of Proposition 33.2.

For the converse, assume that \(\kappa\) is symmetric and that it satisfies the second condition of the proposition. We need to show that \(\kappa\) is a positive definite kernel with respect to complex vectors. If we write \(u_k = a_k + ib_k\), then
\[
u^*K_S u = \sum_{j,k=1}^p \kappa(x_j, x_k)(a_j + ib_j)(a_k - ib_k)
\]
\[
= \sum_{j,k=1}^p (a_ja_k + b_jb_k)\kappa(x_j, x_k) + i \sum_{j,k=1}^p (b_ja_k - a_jb_k)\kappa(x_j, x_k)
\]
\[
= \sum_{j,k=1}^p (a_ja_k + b_jb_k)\kappa(x_j, x_k) + i \sum_{1 \leq j < k \leq p} b_ja_k(\kappa(x_j, x_k) - \kappa(x_k, x_j)).
\]
Thus \(u^*K_S u\) is real iff \(K_S\) is symmetric. \(\Box\)
Consequently we make the following definition.

**Definition 16.3.** Let $X$ be a nonempty set. A function $\kappa : X \times X \to \mathbb{R}$ is a (real) positive definite kernel if $\kappa(x, y) = \kappa(y, x)$ for all $x, y \in X$, and for every finite subset $S = \{x_1, \ldots, x_p\}$ of $X$, if $K_S$ is the $p \times p$ real symmetric matrix

$$K_S = (\kappa(x_i, x_j))_{1 \leq i, j \leq p},$$

then we have

$$u^\top K_S u = \sum_{i,j=1}^{p} \kappa(x_i, x_j)u_iu_j \geq 0, \quad \text{for all } u \in \mathbb{R}^p.$$

Among other things, the next proposition shows that a positive definite kernel satisfies the Cauchy–Schwarz inequality.

**Proposition 16.4.** A hermitian $2 \times 2$ matrix

$$A = \begin{pmatrix} a & \bar{b} \\ b & d \end{pmatrix}$$

is positive semidefinite if and only if $a \geq 0$, $d \geq 0$, and $ad - |b|^2 \geq 0$.

Let $\kappa : X \times X \to \mathbb{C}$ be a positive definite kernel. For all $x, y \in X$, we have

$$|\kappa(x, y)|^2 \leq \kappa(x, x)\kappa(y, y).$$

**Proof.** For all $x, y \in \mathbb{C}$, we have

$$(\bar{x} \quad \bar{y}) \begin{pmatrix} a & \bar{b} \\ b & d \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = (\bar{x} \quad \bar{y}) \begin{pmatrix} ax + \bar{b}y \\ bx + dy \end{pmatrix} = a|x|^2 + bxy + \bar{bxy} + d|y|^2.$$

If $A$ is positive semidefinite, then we already know that $a \geq 0$ and $d \geq 0$. If $a = 0$, then we must have $b = 0$, since otherwise we can make $bxy + \bar{bxy}$, which is twice the real part of $bxy$, as negative as we want. In this case, $ad - |b|^2 = 0$.

If $a > 0$, then

$$a|x|^2 + bxy + \bar{bxy} + d|y|^2 = a \left| x + \frac{\bar{b}}{a}y \right|^2 + \frac{|y|^2}{a} (ad - |b|^2).$$

If $ad - |b|^2 < 0$, we can pick $y \neq 0$ and $x = -(\bar{b}y)/a$, so that the above expression is negative. Therefore, $ad - |b|^2 \geq 0$. The converse is trivial.

If $x = y$, the inequality $|\kappa(x, y)|^2 \leq \kappa(x, x)\kappa(y, y)$ is trivial. If $x \neq y$, the inequality follows by applying the criterion for being positive semidefinite to the matrix

$$\begin{pmatrix} \kappa(x, x) & \kappa(x, y) \\ \kappa(x, y) & \kappa(y, y) \end{pmatrix},$$

as claimed. □
The following property due to I. Schur (1911) shows that the pointwise product of two positive definite kernels is also a positive definite kernel.

**Proposition 16.5.** (I. Schur) If $\kappa_1: X \times X \rightarrow \mathbb{C}$ and $\kappa_2: X \times X \rightarrow \mathbb{C}$ are two positive definite kernels, then the function $\kappa: X \times X \rightarrow \mathbb{C}$ given by $\kappa(x, y) = \kappa_1(x, y)\kappa_2(x, y)$ for all $x, y \in X$ is also a positive definite kernel.

**Proof.** It suffices to prove that if $A = (a_{jk})$ and $B = (b_{jk})$ are two hermitian positive semidefinite $p \times p$ matrices, then so is their pointwise product $C = A \circ B = (a_{jk}b_{jk})$ (also known as Hadamard or Schur product). Recall that a hermitian positive semidefinite matrix $A$ can be diagonalized as $A = U\Lambda U^*$, where $\Lambda$ is a diagonal matrix with nonnegative entries and $U$ is a unitary matrix. Let $\Lambda^{1/2}$ be the diagonal matrix consisting of the positive square roots of the diagonal entries in $\Lambda$. Then we have

$$A = U\Lambda U^* = U\Lambda^{1/2}\Lambda^{1/2}U^* = U\Lambda^{1/2}(U\Lambda^{1/2})^*.$$ 

Thus if we set $R = U\Lambda^{1/2}$, we have

$$A = RR^*,$$

which means that

$$a_{jk} = \sum_{h=1}^{p} r_{jh}r_{kh}.$$ 

Then for any $u \in \mathbb{C}^p$, we have

$$u^*(A \circ B)u = \sum_{j,k=1}^{p} a_{jk}b_{jk}u_j\overline{u_k}$$

$$= \sum_{j,k=1}^{p} \sum_{h=1}^{p} r_{jh}r_{kh}b_{jk}u_j\overline{u_k}$$

$$= \sum_{h=1}^{p} \sum_{j,k=1}^{p} b_{jk}u_jr_{jh}u_kr_{kh}.$$ 

Since $B$ is positive semidefinite, for each fixed $h$, we have

$$\sum_{j,k=1}^{p} b_{jk}u_jr_{jh}u_kr_{kh} = \sum_{j,k=1}^{p} b_{jk}z_j\overline{z_k} \geq 0,$$

as we see by letting $z = (u_1r_{1h}, \ldots, u_pr_{ph})$. 

In contrast, the ordinary product $AB$ of two symmetric positive semidefinite matrices $A$ and $B$ may not be symmetric positive semidefinite; see Section 6.8 for an example.

Here are other ways of obtaining new positive definite kernels from old ones.
**Proposition 16.6.** Let $\kappa_1: X \times X \to \mathbb{C}$ and $\kappa_2: X \times X \to \mathbb{C}$ be two positive definite kernels, $f: X \to \mathbb{C}$ be a function, $\psi: X \to \mathbb{R}^N$ be a function, $\kappa_3: \mathbb{R}^N \times \mathbb{R}^N \to \mathbb{C}$ be a positive definite kernel, and $a \in \mathbb{R}$ be any positive real. Then the following functions are positive definite kernels:

1. $\kappa(x, y) = \kappa_1(x, y) + \kappa_2(x, y)$.
2. $\kappa(x, y) = a\kappa_1(x, y)$.
3. $\kappa(x, y) = f(x)f(y)$.
4. $\kappa(x, y) = \kappa_3(\psi(x), \psi(y))$.
5. If $B$ is a symmetric positive semidefinite $n \times n$ matrix, then the map $\kappa: \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ given by $\kappa(x, y) = x^\top By$ is a positive definite kernel.

**Proof.**

1. For every finite subset $S = \{x_1, \ldots, x_p\}$ of $X$, if $K_1$ is the $p \times p$ matrix

$$K_1 = (\kappa_1(x_k, x_j))_{1 \leq j, k \leq p}$$

and if if $K_2$ is the $p \times p$ matrix

$$K_2 = (\kappa_2(x_k, x_j))_{1 \leq j, k \leq p},$$

then for any $u \in \mathbb{C}^p$, we have

$$u^\top (K_1 + K_2)u = u^\top K_1u + u^\top K_2u \geq 0,$$

since $u^\top K_1u \geq 0$ and $u^\top K_2u \geq 0$ because $\kappa_2$ and $\kappa_2$ are positive definite kernels, which means that $K_1$ and $K_2$ are positive semidefinite.

2. We have

$$u^\top (aK_1)u = au^\top K_1u \geq 0,$$

since $a > 0$ and $u^\top K_1u \geq 0$.

3. For every finite subset $S = \{x_1, \ldots, x_p\}$ of $X$, if $K$ is the $p \times p$ matrix

$$K = (\kappa(x_k, x_j))_{1 \leq j, k \leq p} = (f(x_k)f(x_j))_{1 \leq j, k \leq p}$$

then we have

$$u^\top Ku = \sum_{j,k=1}^p \kappa(x_j, x_k)u_j\overline{u_k} = \sum_{j,k=1}^p u_jf(x_j)\overline{u_kf(x_k)} = \left| \sum_{j=1}^p u_jf(x_j) \right|^2 \geq 0.$$
16.1. BASIC PROPERTIES OF POSITIVE DEFINITE KERNELS

(4) For every finite subset \( S = \{x_1, \ldots, x_p\} \) of \( X \), the \( p \times p \) matrix \( K \) given by
\[
K = (\kappa(x_k, x_j))_{1\leq j, k \leq p} = (\kappa_3(\psi(x_k), \psi(x_j)))_{1\leq j, k \leq p}
\]
is symmetric positive semidefinite since \( \kappa_3 \) is a positive definite kernel.

(5) As in the proof of Proposition 33.5 (adapted to the real case) there is a matrix \( R \) such that
\[
B = RR^\top,
\]
so
\[
\kappa(x, y) = x^\top By = x^\top RR^\top y = (R^\top x)^\top R^\top y = \langle R^\top x, R^\top y \rangle,
\]
so \( \kappa \) is the kernel function given by the feature map \( \varphi(x) = R^\top x \) from \( \mathbb{R}^n \) to itself, and by Proposition 33.1, it is a symmetric positive definite kernel. \( \square \)

**Proposition 16.7.** Let \( \kappa_1: X \times X \to \mathbb{C} \) be a positive definite kernel, and let \( p(z) \) be a polynomial with nonnegative coefficients. Then the following functions \( \kappa \) defined below are also positive definite kernels.

1. \( \kappa(x, y) = p(\kappa_1(x, y)) \).
2. \( \kappa(x, y) = e^{\kappa_1(x, y)} \).
3. If \( X \) is real Hilbert space with inner product \( \langle -, - \rangle_X \) and corresponding norm \( \| - \|_X \),
   \[
   \kappa(x, y) = e^{-\frac{\|x-y\|^2_2}{2\sigma^2}}
   \]
   for any \( \sigma > 0 \).

**Proof.** (1) If \( p(z) = a_m z^m + \cdots + a_1 z + a_0 \), then
\[
p(\kappa_1(x, y)) = a_m \kappa_1(x, y)^m + \cdots + a_1 \kappa_1(x, y) + a_0.
\]
Since \( a_k \geq 0 \) for \( k = 0, \ldots, m \), by Proposition 33.5 and Proposition 33.6(2), each function \( a_k \kappa_1(x, y)^k \) with \( 1 \leq k \leq m \) is a positive definite kernel, by Proposition 33.6(3) with \( f(x) = \sqrt{a_0} \), the constant function \( a_0 \) is a positive definite kernel, and by Proposition 33.6(1), \( p(\kappa_1(x, y)) \) is a positive definite kernel.

(2) We have
\[
e^{\kappa_1(x, y)} = \sum_{k=0}^{\infty} \frac{\kappa_1(x, y)^k}{k!}.
\]
By (1), the partial sums
\[
\sum_{k=0}^{m} \frac{\kappa_1(x, y)^k}{k!}
\]
are positive definite kernels, and since \( e^{\kappa_1(x,y)} \) is the (uniform) pointwise limit of positive definite kernels, it is also a positive definite kernel.

(3) By Proposition 33.6(2), since the map \((x, y) \mapsto \langle x, y \rangle_X\) is obviously a positive definite kernel (the feature map is the identity) and since \( \sigma \neq 0 \), the function \((x, y) \mapsto \langle x, y \rangle_X / \sigma^2\) is a positive definite kernel, so by (2),

\[
\kappa_1(x, y) = e^{\langle x, y \rangle_X / \sigma^2}
\]

is a positive definite kernel. Let \( f : X \to \mathbb{R} \) be the function given by

\[
f(x) = e^{-\|x\|^2 / 2\sigma^2}.
\]

Then by Proposition 33.6(3),

\[
\kappa_2(x, y) = f(x)f(y) = e^{-\|x\|^2 / 2\sigma^2} e^{-\|y\|^2 / 2\sigma^2} = e^{-\|x\|^2_2 + \|y\|^2_2 / 2\sigma^2}
\]

is a positive definite kernel. By Proposition 33.5, the function \( \kappa_1 \kappa_2 \) is a positive definite kernel, that is

\[
\kappa_1(x, y) \kappa_2(x, y) = e^{\langle x, y \rangle_X} e^{-\|x\|^2_2 + \|y\|^2_2 / 2\sigma^2} = \kappa_1(x, x) - \kappa_1(y, y) + 2 \kappa_1(x, y)
\]

is a positive definite kernel. 

The positive definite kernel

\[
\kappa(x, y) = e^{-\|x-y\|^2_2 / 2\sigma^2}
\]

is called a Gaussian kernel. This kernel requires a feature map in an infinite-dimensional space because it is an infinite sum of distinct kernels.

**Remark:** If \( \kappa_1 \) is a positive definite kernel, the proof of Proposition 33.7(3) is immediately adapted to show that

\[
\kappa(x, y) = e^{-\kappa_1(x, x) + \kappa_1(y, y) - 2\kappa_1(x, y) / 2\sigma^2}
\]

is a positive definite kernel.

Next we prove that every positive definite kernel arises from a feature map in a Hilbert space which is a function space.

### 16.2 Hilbert Space Representation of a Positive Definite Kernel

The following result shows how to construct a so-called reproducing kernel Hilbert space, for short RKHS, from a positive definite kernel.
Theorem 16.8. Let \( \kappa : X \times X \to \mathbb{C} \) be a positive definite kernel on a nonempty set \( X \). For every \( x \in X \), let \( \kappa_x : X \to \mathbb{C} \) be the function given by

\[
\kappa_x(y) = \kappa(x, y), \quad y \in X.
\]

Let \( H_0 \) be the subspace of the vector space \( \mathbb{C}^X \) of functions from \( X \) to \( \mathbb{C} \) spanned by the family of functions \( (\kappa_x)_{x \in X} \), and let \( \varphi : X \to H_0 \) be the map given by \( \varphi(x) = \kappa_x \). There is a hermitian inner product \( \langle -,- \rangle \) on \( H_0 \) such that

\[
\kappa(x, y) = \langle \varphi(x), \varphi(y) \rangle, \quad \text{for all } x, y \in X.
\]

The completion \( H \) of \( H_0 \) is a Hilbert space, and the map \( \eta : H \to \mathbb{C}^X \) given by

\[
\eta(f)(x) = \langle f, \kappa_x \rangle, \quad x \in X,
\]

is linear and injective, so \( H \) can be identified with a subspace of \( \mathbb{C}^X \). We also have

\[
\kappa(x, y) = \langle \varphi(x), \varphi(y) \rangle, \quad \text{for all } x, y \in X.
\]

For all \( f \in H_0 \) and all \( x \in X \),

\[
\langle f, \kappa_x \rangle = f(x),
\]

a property known as the **reproducing property**.

Proof. For any two linear combinations \( f = \sum_{j=1}^{p} \alpha_j \kappa_{x_j} \) and \( g = \sum_{k=1}^{q} \beta_k \kappa_{y_k} \) in \( H_0 \), with \( x_j, y_k \in X \) and \( \alpha_j, \beta_k \in \mathbb{C} \), define \( \langle f, g \rangle \) by

\[
\langle f, g \rangle = \sum_{j=1}^{p} \sum_{k=1}^{q} \alpha_j \beta_k \kappa(x_j, y_k). \quad (\dagger)
\]

At first glance, the above expression appears to depend on the expression of \( f \) and \( g \) as linear combinations, but since \( \kappa(x_j, y_k) = \kappa(y_k, x_j) \), observe that

\[
\sum_{k=1}^{q} \beta_k f(y_k) = \sum_{j=1}^{p} \sum_{k=1}^{q} \alpha_j \beta_k \kappa(x_j, y_k) = \sum_{j=1}^{p} \alpha_j g(x_j), \quad (\star)
\]

and since the first and the third term are equal for all linear combinations representing \( f \) and \( g \), we conclude that \( (\dagger) \) depends only on \( f \) and \( g \) and not on their representation as a linear combination.

Obviously \( (\dagger) \) defines a hermitian sequilinear form. For every \( f \in H_0 \), we have

\[
\langle f, f \rangle = \sum_{j,k=1}^{p} \alpha_j \beta_k \kappa(x_j, x_k) \geq 0,
\]
since $\kappa$ is a positive definite kernel. For any finite subset \( \{f_1, \ldots, f_n\} \) of $H_0$ and any $z \in \mathbb{C}^n$, we have

\[
\sum_{j,k=1}^{n} \langle f_j, f_k \rangle z_j \overline{z_k} = \left\langle \sum_{j=1}^{n} z_j f_j, \sum_{j=1}^{n} z_j f_j \right\rangle \geq 0,
\]

which shows that the map $(f, g) \mapsto \langle f, g \rangle$ from $H_0 \times H_0$ to $\mathbb{C}$ is a positive definite kernel.

Observe that for all $f \in H_0$ and all $x \in X$, (†) implies that

\[
\langle f, \kappa_x \rangle = \sum_{j=1}^{k} \alpha_j \kappa(x_j, x) = f(x),
\]

a property known as the reproducing property. The above implies that

\[
\langle \kappa_x, \kappa_y \rangle = \kappa(x, y). \tag{**}
\]

By Proposition 33.4 applied to the positive definite kernel $(f, g) \mapsto \langle f, g \rangle$, we have

\[
|\langle f, \kappa_x \rangle|^2 \leq \langle f, f \rangle \langle \kappa_x, \kappa_x \rangle,
\]

that is,

\[
|f(x)|^2 \leq \langle f, f \rangle \kappa(x, x),
\]

so $\langle f, f \rangle = 0$ implies that $f(x) = 0$ for all $x \in X$, which means that $\langle -, - \rangle$ as defined by (†) is positive definite. Therefore, $\langle -, - \rangle$ is a hermitian inner product on $H_0$, and by (**) and since $\varphi(x) = \kappa_x$, we have

\[
\kappa(x, y) = \langle \varphi(x), \varphi(y) \rangle, \quad \text{for all } x, y \in X.
\]

Let $H$ be the Hilbert space which is the completion of $H_0$, so that $H_0$ is dense in $H$. The map $\eta: H \to \mathbb{C}^X$ given by

\[
\eta(f)(x) = \langle f, \kappa_x \rangle
\]

is obviously linear, and it is injective because the family $(\kappa_x)_{x \in X}$ spans $H_0$ which is dense in $H$, thus it is also dense in $H$, so if $\langle f, \kappa_x \rangle = 0$ for all $x \in X$, then $f = 0$.

If we identify a function $f \in H$ with the function $\eta(f)$, then we have the reproducing property

\[
\langle f, \kappa_x \rangle = f(x), \quad \text{for all } f \in H \text{ and all } x \in X.
\]

If $X$ is finite, then $\mathbb{C}^X$ is finite-dimensional. If $X$ is a separable topological space and if $\kappa$ is continuous, then it can be shown that $H$ is a separable Hilbert space.

Also, if $\kappa: X \times X \to \mathbb{R}$ is a real symmetric positive definite kernel, then we see immediately that Theorem 33.8 holds with $H_0$ a real Euclidean space and $H$ a real Hilbert space.
Remark: If \( X = G \), where \( G \) is a locally compact group, then a function \( p : G \to \mathbb{C} \) (not necessarily continuous) is positive semidefinite if for all \( s_1, \ldots, s_n \in G \) and all \( \xi_1, \ldots, \xi_n \in \mathbb{C} \), we have
\[
\sum_{j,k=1}^n p(s_j^{-1}s_k)\bar{\xi}_k\xi_j \geq 0.
\]
So if we define \( \kappa : G \times G \to \mathbb{C} \) by
\[
\kappa(s,t) = p(t^{-1}s),
\]
then \( \kappa \) is a positive definite kernel on \( G \). If \( p \) is continuous, then it is known that \( p \) arises from a unitary representation \( U : G \to U(H) \) of the group \( G \) in a Hilbert space \( H \) with inner product \( \langle \cdot, \cdot \rangle \) (a homomorphism with a certain continuity property), in the sense that there is some vector \( x_0 \in H \) such that
\[
p(s) = \langle U(s)(x_0), x_0 \rangle, \quad \text{for all } s \in G.
\]
Since the \( U(s) \) are unitary operators on \( H \),
\[
p(t^{-1}s) = \langle U(t^{-1}s)(x_0), x_0 \rangle = \langle U(t^{-1})(U(s)(x_0)), x_0 \rangle = \langle U(t)(U(s)(x_0)), x_0 \rangle = \langle U(s)(x_0), U(t)(x_0) \rangle,
\]
which shows that
\[
\kappa(s,t) = \langle U(s)(x_0)), U(t)(x_0) \rangle,
\]
so the map \( \varphi : G \to H \) given by
\[
\varphi(s) = U(s)(x_0)
\]
is a feature map into the feature space \( H \). This theorem is due to Gelfand and Raikov (1943).

The proof of Theorem 33.8 is essentially identical to part of Godement’s proof of the above result about the correspondence between functions of positive type and unitary representations; see Helgason [55], Chapter IV, Theorem 1.5. Theorem 33.8 is a little more general since it does not assume that \( X \) is a group, but when \( G \) is a group, the feature map arises from a unitary representation.

Kernels on collections of sets can be defined in terms of measures.

Example 16.7. Let \((D, \mathcal{A})\) be a measurable space, where \( D \) is a nonempty set and \( \mathcal{A} \) is a \( \sigma \)-algebra on \( D \) (the measurable sets). Let \( X \) be a subset of \( \mathcal{A} \). If \( \mu \) is a positive measure on \((D, \mathcal{A})\) and if \( \mu \) is finite, which means that \( \mu(D) \) is finite, then we can define the map \( \kappa_1 : X \times X \to \mathbb{R} \) given by
\[
\kappa_1(A_1, A_2) = \mu(A_1 \cap A_2), \quad A_1, A_2 \in X.
\]
We can show that \( \kappa \) is a kernel function as follows. Let \( H = L^2_\mu(D, \mathcal{A}, \mathbb{R}) \) be the Hilbert space of \( \mu \)-square-integrable functions, with the inner product
\[
\langle f, g \rangle = \int_D f(s)g(s) \, d\mu(s),
\]
and let \( \varphi: X \rightarrow H \) be the feature embedding given by
\[
\varphi(A) = \chi_A, \quad A \in X,
\]
the characteristic function of \( A \). Then we have
\[
\kappa_1(A_1, A_2) = \mu(A_1 \cap A_2) = \int_D \chi_{A_1 \cap A_2}(s) d\mu(s) \\
= \int_D \chi_{A_1}(s) \chi_{A_2}(s) d\mu(s) = \langle \chi_{A_1}, \chi_{A_2} \rangle \\
= \langle \varphi(A_1), \varphi(A_2) \rangle.
\]

The above kernel is called the intersection kernel. If we assume that \( \mu \) is normalized so that \( \mu(D) = 1 \), then we also have the union complement kernel:
\[
\kappa_2(A_1, A_2) = \mu(A_1 \cap \overline{A_2}) = 1 - \mu(A_1 \cup A_2).
\]

The sum \( \kappa_3 \) of the kernels \( \kappa_1 \) and \( \kappa_2 \) is the agreement kernel:
\[
\kappa_3(A_1, A_2) = 1 - \mu(A_1 - A_2) - \mu(A_2 - A_1).
\]

Many other kinds of kernels can be designed, in particular, graph kernels. For comprehensive presentations of kernels, see Schölkopf and Smola [86] and Shawe–Taylor and Christianini [97].

### 16.3 Kernel PCA

As an application of kernel functions, we discuss a generalization of the method of principal component analysis (PCA). Suppose we have a set of data \( S = \{x_1, \ldots, x_n\} \) in some input space \( \mathcal{X} \), and pretend that we have an embedding \( \varphi: \mathcal{X} \rightarrow F \) of \( \mathcal{X} \) in a (real) feature space \( (F, \langle -,- \rangle) \), but that we only have access to the kernel function \( \kappa(x,y) = \langle \varphi(x), \varphi(y) \rangle \). We would like to do PCA analysis on the set \( \varphi(S) = \{\varphi(x_1), \ldots, \varphi(x_n)\} \).

There are two obstacles:

1. We need to center the data and compute the inner products of pairs of centered data. More precisely, if the centroid of \( \varphi(S) \) is
\[
\mu = \frac{1}{n}(\varphi(x_1) + \cdots + \varphi(x_n)),
\]
then we need to compute the inner products \( \langle \varphi(x) - \mu, \varphi(y) - \mu \rangle \).
Let us assume that $F = \mathbb{R}^d$ with the standard Euclidean inner product and that the data points $\varphi(x_i)$ are expressed as row vectors $X_i$ of an $n \times d$ matrix $X$ (as it is customary). Then the inner products $\kappa(x_i, x_j) = \langle \varphi(x_i), \varphi(x_j) \rangle$ are given by the kernel matrix $K = XX^T$. Be aware that with this representation, $\varphi(x_i)$ is a $d$-dimensional column vector and that $\varphi(x_i) = X_i^\top$. However, the $j$th component $(Y_k)_j$ of the principal component $Y_k$ (viewed as a $n$-dimensional column vector) is given by the projection of $\hat{X}_j = X_j - \mu$ onto the direction $u_k$ (viewing $\mu$ as a $d$-dimensional row vector), which is a unit eigenvector of the matrix $(X - \mu)^\top(X - \mu)$ (where $\hat{X} = X - \mu$ is the matrix whose $j$th row is $\hat{X}_j = X_j - \mu$), is given by the inner product

$$\langle X_j - \mu, u_k \rangle = (Y_k)_j;$$

see Definition 17.2 and Theorem 17.11. The problem is that we know what the matrix $(X - \mu)(X - \mu)^\top$ is from (1), because it can be expressed in terms of $K$, but we don’t know what $(X - \mu)^\top(X - \mu)$ is, because we don’t have access to $\hat{X} = X - \mu$.

Both difficulties are easily overcome. For (1), we have

$$\langle \varphi(x) - \mu, \varphi(y) - \mu \rangle = \left( \varphi(x) - \frac{1}{n} \sum_{k=1}^{n} \varphi(x_k), \varphi(y) - \frac{1}{n} \sum_{k=1}^{n} \varphi(x_k) \right) = \kappa(x, y) - \frac{1}{n} \sum_{i=1}^{n} \kappa(x, x_i) - \frac{1}{n} \sum_{j=1}^{n} \kappa(x_j, y) + \frac{1}{n^2} \sum_{i,j=1}^{n} \kappa(x_i, x_j).$$

For (2), if $K$ is the kernel matrix $K = (\kappa(x_i, x_j))$, then the kernel matrix $\hat{K}$ corresponding to the kernel function $\hat{\kappa}$ given by

$$\hat{\kappa}(x, y) = \langle \varphi(x) - \mu, \varphi(y) - \mu \rangle$$

can be expressed in terms of $K$. Let $1$ be the column vector (of dimension $n$) whose entries are all 1. Then $11^\top$ is the $n \times n$ matrix whose entries are all 1. If $A$ is an $n \times n$ matrix, then $1^\top A$ is the row vector consisting of the sums of the columns of $A$, $A 1$ is the column vector consisting of the sums of the rows of $A$, and $1^\top A 1$ is the sum of all the entries in $A$. Then it is easy to see that the kernel matrix corresponding to the kernel function $\hat{\kappa}$ is given by

$$\hat{K} = K - \frac{1}{n} 1 1^\top K - \frac{1}{n} K 1 1^\top + \frac{1}{n^2} (1^\top K 1) 1 1^\top.$$

Suppose $\hat{X} = X - \mu$ has rank $r$. To overcome the second problem, note that if $\hat{X} = VDU^\top$

is an SVD for $\hat{X}$, then

$$\hat{X}^\top = UD^\top V^\top.$$
is an SVD for $\hat{X}^\top$, and the $r \times r$ submatrix of $D^T$ consisting of the first $r$ rows and $r$ columns of $D^\top$ (and $D$), is the diagonal $\Sigma^r$ matrix consisting of the singular values $\sigma_1 \geq \cdots \geq \sigma_r$ of $\hat{X}$, so we can express the matrix $U_r$ consisting of the first $r$ columns $u_k$ of $U$ in terms of the matrix $V_r$ consisting of the first $r$ columns $v_k$ of $V$ $(1 \leq k \leq r)$ as

$$U_r = \hat{X}^\top V_r \Sigma_r^{-1}.$$  

Furthermore, $\sigma_1^2 \geq \cdots \geq \sigma_r^2$ are the nonzero eigenvalues of $\hat{K} = \hat{X} \hat{X}^\top$, and the columns of $V_r$ are corresponding unit eigenvectors of $\hat{K}$. From

$$U_r = \hat{X}^\top V_r \Sigma_r^{-1}$$

the $k$th column $u_k$ of $U_r$ (which is a unit eigenvector of $\hat{X}^\top \hat{X}$ associated with the eigenvalue $\sigma_k^2$) is given by

$$u_k = \sum_{i=1}^{n} \sigma_k^{-1}(v_k)_i \hat{X}_i = \sum_{i=1}^{n} \sigma_k^{-1}(v_k)_i \varphi(x_i), \quad 1 \leq k \leq r,$$

so the projection of $\varphi(x)$ onto $u_k$ is given by

$$\langle \varphi(x), u_k \rangle = \left( \varphi(x), \sum_{i=1}^{n} \sigma_k^{-1}(v_k)_i \varphi(x_i) \right) = \sum_{i=1}^{n} \sigma_k^{-1}(v_k)_i \langle \varphi(x), \varphi(x_i) \rangle = \sum_{i=1}^{n} \sigma_k^{-1}(v_k)_i \hat{K}(x, x_i).$$

Therefore, the $j$th component of the principal component $Y_k$ in the principal direction $u_k$ is given by

$$(Y_k)_j = \langle X_j - \mu, u_k \rangle = \sum_{i=1}^{n} \sigma_k^{-1}(v_k)_i \hat{K}(x_j, x_i) = \sum_{i=1}^{n} \sigma_k^{-1}(v_k)_i \hat{K}_{ij}.$$

The generalization of kernel PCA to a general embedding $\varphi: \mathcal{X} \to F$ of $\mathcal{X}$ in a (real) feature space $(F, \langle - , - \rangle)$ with the kernel matrix $K$ given by

$$K_{ij} = \langle \varphi(x_i), \varphi(x_j) \rangle,$$

goess as follows. Let $r$ be the rank of $\hat{K}$, where

$$\hat{K} = K - \frac{1}{n} 1^\top K 1 + \frac{1}{n} K 1^\top 1 + \frac{1}{n^2} (1^\top K 1) 1 1^\top,$$

let $\sigma_1^2 \geq \cdots \geq \sigma_r^2$ be the nonzero eigenvalues of $\hat{K}$, and let $v_1, \ldots, v_r$ be corresponding unit eigenvectors. The notation

$$\alpha_k = \sigma_k^{-1} v_k$$
16.4 \( \nu \)-SV Regression

is often used, where the \( \alpha_k \) are called the dual variables. The column vector \( Y_k \) (\( 1 \leq k \leq r \)) defined by

\[
Y_k = \left( \sum_{i=1}^{n} (\alpha_k)_{ij} \tilde{K}_{ij} \right)_{j=1}^{n}
\]

is called the \( k \)th kernel principal component (for short \( k \)th kernel PCA) of the data set \( S = \{x_1, \ldots, x_n\} \) in the direction \( u_k = \sum_{i=1}^{n} \sigma_k^{-1}(v_k)_i \tilde{X}_i^\top \) (even though the matrix \( \tilde{X} \) is not known).

In the next section, we give another illustration of the use of kernel functions in a generalization of ridge regression (see Section 32.1).

16.4 \( \nu \)-SV Regression

Let \( \{(x_1, y_1), \ldots, (x_m, y_m)\} \) be a set of observed data usually called a set of training data, with \( x_i \in \mathbb{R}^n \) and \( y_i \in \mathbb{R} \). Our goal is to learn an affine function \( f \) of the form \( f(x) = w^\top x - b \) that fits the set of training data, but does not penalize errors below some given \( \epsilon \geq 0 \). Thus we try to fit a tube with radius \( \epsilon \) to the data, but we also allow errors, in the sense that some data \( x_i \) may satisfy the equality \( f(x_i) - y_i = \epsilon + \xi_i \) for some \( \xi_i > 0 \), or the equality \(- (f(x_i) - y_i) = \epsilon + \xi'_i \) for some \( \xi'_i > 0 \). In this case, \( x_i \) lies outside of the tube with radius \( \epsilon \).

The trade off between the size of \( \epsilon \) and the size of the slack variables \( \xi_i \) and \( \xi'_i \) is achieved by using two constants \( \nu \geq 0 \) and \( C > 0 \). The method of \( \nu \)-support vector regression, for short \( \nu \)-SV regression, is specified by the following minimization problem:

\( \nu \)-SV Regression:

\[
\text{minimize } \frac{1}{2} w^\top w + C \left( \nu \epsilon + \frac{1}{m} \sum_{i=1}^{m} (\xi_i + \xi'_i) \right)
\]

subject to

\[
\begin{align*}
  w^\top x_i - b - y_i & \leq \epsilon + \xi_i, \quad \xi_i \geq 0, \quad i = 1, \ldots, m \\
  -w^\top x_i + b + y_i & \leq \epsilon + \xi'_i, \quad \xi'_i \geq 0, \quad i = 1, \ldots, m \\
  \epsilon & \geq 0,
\end{align*}
\]

minimizing over the variables \( w, b, \epsilon, \xi, \) and \( \xi' \). The constraints are affine.

First, observe that the equations

\[
\begin{align*}
  w^\top x_i - b - y_i &= \epsilon + \xi_i \\
  -w^\top x_i + b + y_i &= \epsilon + \xi'_i
\end{align*}
\]

can only hold simultaneously if

\[
\epsilon + \xi_i = -\epsilon - \xi'_i,
\]
that is,

\[ 2\epsilon + \xi_i + \xi'_i = 0, \]

and since \( \epsilon, \xi_i, \xi'_i \geq 0 \), this can happen only if \( \epsilon = \xi_i = \xi'_i = 0 \), and then

\[ w^\top x_i - b = y_i. \]

In particular, if \( \epsilon > 0 \), then the equations

\[ w^\top x_i - b - y_i = \epsilon + \xi_i \]
\[ -w^\top x_i + b + y_i = \epsilon + \xi'_i \]

cannot hold simultaneously. Also, since \( -w^\top x_i + b + y_i = -(w^\top x_i - b - y_i) \), for an optimal solution, if \( w^\top x_i - b - y_i \geq 0 \), then \( \xi'_i = 0 \) since the inequality

\[ -w^\top x_i + b + y_i \leq \epsilon + \xi'_i \]

is trivially satisfied (because \( \epsilon, \xi'_i \geq 0 \)), and if \( w^\top x_i - b - y_i \leq 0 \), then similarly \( \xi_i = 0 \). Therefore, we have the equations

\[ \xi_i\xi'_i = 0, \quad i = 1, \ldots, m. \]

Observe that if \( \nu > 1 \), then an optimal solution of the above program must yield \( \epsilon = 0 \). Indeed, if \( \epsilon > 0 \), we can reduce it by a small amount \( \delta > 0 \) and increase \( \xi_i + \xi'_i \) by \( \delta \) to still satisfy the constraints, but the objective function changes by the amount \( -\nu\delta + \delta \), which is negative since \( \nu > 1 \), so \( \epsilon > 0 \) is not optimal.

Driving \( \epsilon \) to zero is not the intended goal, because typically the data is not noise free so very few pairs \( (x_i, y_i) \) will satisfy the equation \( w^\top x_i - b = y_i \), and then many pair \( (x_i, y_i) \) will correspond to an error (\( \xi_i > 0 \) or \( \xi'_i > 0 \)). Thus, typically we assume that \( 0 < \nu \leq 1 \).

To construct the Lagrangian, we assign Lagrange multipliers \( \alpha_i \geq 0 \) to the constraints \( w^\top x_i - b - y_i \leq \epsilon + \xi_i \), Lagrange multipliers \( \alpha'_i \geq 0 \) to the constraints \( -w^\top x_i + b + y_i \leq \epsilon + \xi'_i \), Lagrange multipliers \( \eta_i \geq 0 \) to the constraints \( \xi_i \geq 0 \), Lagrange multipliers \( \eta'_i \geq 0 \) to the constraints \( \xi'_i \geq 0 \), and the Lagrange multiplier \( \beta \geq 0 \) to the constraint \( \epsilon \geq 0 \). The Lagrangian is

\[
L(w, b, \alpha, \alpha', \beta, \xi, \xi', \epsilon, \eta, \eta') = \frac{1}{2} w^\top w + C \left( \nu \epsilon + \frac{1}{m} \sum_{i=1}^{m} (\xi_i + \xi'_i) \right) \\
- \beta \epsilon - \sum_{i=1}^{m} (\eta_i \xi_i + \eta'_i \xi'_i) \\
+ \sum_{i=1}^{m} \alpha_i (w^\top x_i - b - y_i - \epsilon - \xi_i) \\
+ \sum_{i=1}^{m} \alpha'_i (-w^\top x_i + b + y_i - \epsilon - \xi'_i),
\]
The Lagrangian can also be written as

\[
L(w, b, \alpha, \alpha', \beta, \xi, \xi', \epsilon, \eta, \eta') = \frac{1}{2} w^\top w + w^\top \left( \sum_{i=1}^{m} (\alpha_i - \alpha'_i) x_i \right) \\
+ \epsilon \left( C \nu - \beta - \sum_{i=1}^{m} (\alpha_i + \alpha'_i) \right) \\
+ \sum_{i=1}^{m} \xi_i \left( \frac{C}{m} - \alpha_i - \eta_i \right) + \sum_{i=1}^{m} \xi'_i \left( \frac{C}{m} - \alpha'_i - \eta'_i \right) \\
- b \left( \sum_{i=1}^{m} (\alpha_i - \alpha'_i) \right) - \sum_{i=1}^{m} (\alpha_i - \alpha'_i) y_i.
\]

To find the dual function \(G(\alpha, \alpha', \eta, \eta', \beta)\), we minimize \(L(w, b, \alpha, \alpha', \beta, \xi, \xi', \epsilon, \eta, \eta')\) with respect to the primal variables \(w, \epsilon, b, \xi\) and \(\xi'\). Observe that the Lagrangian is convex, and since \((w, \epsilon, \xi, \xi') \in \mathbb{R}^n \times \mathbb{R} \times \mathbb{R}^m \times \mathbb{R}^m\), a convex open set, by Theorem 21.11, the Lagrangian has a minimum iff \(\nabla L_{w,\epsilon,b,\xi,\xi'} = 0\), so we compute the gradient \(\nabla L_{w,\epsilon,b,\xi,\xi'}\). We obtain

\[
\nabla L_{w,\epsilon,b,\xi,\xi'} = \begin{pmatrix}
w + \sum_{i=1}^{m} (\alpha_i - \alpha'_i) x_i \\
C \nu - \beta - \sum_{i=1}^{m} (\alpha_i + \alpha'_i) \\
\sum_{i=1}^{m} (\alpha_i - \alpha'_i) \\
\frac{C}{m} - \alpha - \eta \\
\frac{C}{m} - \alpha' - \eta'
\end{pmatrix},
\]

where

\[
\left( \frac{C}{m} - \alpha - \eta \right)_i = \frac{C}{m} - \alpha_i - \eta_i, \quad \text{and} \quad \left( \frac{C}{m} - \alpha' - \eta' \right)_i = \frac{C}{m} - \alpha'_i - \eta'_i.
\]

Consequently, if we set \(\nabla L_{w,\epsilon,b,\xi,\xi'} = 0\), we obtain the equations

\[
w = \sum_{i=1}^{m} (\alpha'_i - \alpha_i) x_i, \quad (*_w)
\]

\[
C \nu - \beta - \sum_{i=1}^{m} (\alpha_i + \alpha'_i) = 0
\]

\[
\sum_{i=1}^{m} (\alpha_i - \alpha'_i) = 0
\]

\[
\frac{C}{m} - \alpha - \eta = 0, \quad \frac{C}{m} - \alpha' - \eta' = 0.
\]
Substituting the above equations in the second expression for the Lagrangian, we find that the dual function $G$ is independent of the variables $\beta, \eta, \eta'$ and is given by

$$G(\alpha, \alpha') = -\frac{1}{2} \sum_{i,j=1}^{m} (\alpha'_i - \alpha_i)(\alpha'_j - \alpha_j)x_i^\top x_j - \sum_{i=1}^{m} (\alpha_i - \alpha'_i)y_i$$

if

$$C\nu - \beta - \sum_{i=1}^{m} (\alpha_i + \alpha'_i) = 0$$
$$\sum_{i=1}^{m} (\alpha_i - \alpha'_i) = 0$$
$$\frac{C}{m} - \alpha - \eta = 0, \quad \frac{C}{m} - \alpha' - \eta' = 0,$$

and $-\infty$ otherwise.

The dual program is obtained by maximizing $G(\alpha, \alpha')$ or equivalently by minimizing $-G(\alpha, \alpha')$, over $\alpha, \alpha' \in \mathbb{R}_+^m$. Taking into account the fact that $\eta, \eta' \geq 0$ and $\beta \geq 0$, we obtain the following dual program:

minimize $$\frac{1}{2} \sum_{i,j=1}^{m} (\alpha'_i - \alpha_i)(\alpha'_j - \alpha_j)x_i^\top x_j + \sum_{i=1}^{m} (\alpha_i - \alpha'_i)y_i$$

subject to

$$\sum_{i=1}^{m} (\alpha_i + \alpha'_i) \leq C\nu$$
$$\sum_{i=1}^{m} (\alpha_i - \alpha'_i) = 0$$

$$0 \leq \alpha_i \leq \frac{C}{m}, \quad 0 \leq \alpha'_i \leq \frac{C}{m}, \quad i = 1, \ldots, m.$$

The KKT conditions (for the primal program) are

$$\alpha_i(w^\top x_i - b - y_i - \epsilon - \xi_i) = 0, \quad i = 1, \ldots, m$$
$$\alpha'_i(-w^\top x_i + b + y_i - \epsilon - \xi'_i) = 0, \quad i = 1, \ldots, m$$
$$\beta\epsilon = 0$$
$$\eta_i\xi_i = 0, \quad i = 1, \ldots, m$$
$$\eta'_i\xi'_i = 0, \quad i = 1, \ldots, m.$$
If $\epsilon > 0$, since the equations
\[
\begin{align*}
    w^\top x_i - b - y_i &= \epsilon + \xi_i \\
    -w^\top x_i + b + y_i &= \epsilon + \xi_i'
\end{align*}
\]
cannot hold simultaneously, we must have
\[
    \alpha_i \alpha'_i = 0, \quad i = 1, \ldots, m. \tag{\alpha \alpha'}
\]

From the equations
\[
\begin{align*}
    \frac{C}{m} - \alpha_i - \eta_i &= 0, \quad \frac{C}{m} - \alpha'_i - \eta'_i = 0, \quad \eta_i \xi_i = 0, \quad \eta'_i \xi'_i = 0,
\end{align*}
\]
we get the equations
\[
\left( \frac{C}{m} - \alpha_i \right) \xi_i = 0, \quad \left( \frac{C}{m} - \alpha'_i \right) \xi'_i = 0, \quad i = 1, \ldots, m. \tag{*}
\]

These equations show that if $\xi_i > 0$, then $\alpha_i = \frac{C}{m}$, so we have the active constraint
\[
    w^\top x_i - b - y_i = \epsilon + \xi_i
\]
and $x_i$ is an error, and similarly, if $\xi'_i > 0$, then $\alpha'_i = \frac{C}{m}$, so we have the active constraint
\[
    -w^\top x_i + b + y_i = \epsilon + \xi'_i
\]
and $x_i$ is an error.

If the primal has an optimal solution with $w \neq 0$ and $\epsilon > 0$, then by ($*_w$) and since
\[
\sum_{i=1}^{m} (\alpha_i - \alpha'_i) = 0 \quad \text{and} \quad \alpha_i \alpha'_i = 0,
\]
there is there is some $i_0$ such that $\alpha_{i_0} > 0$ and some $j_0 \neq i_0$ such that $\alpha'_{j_0} > 0$. Under the mild hypothesis that there is some $i_0$ such that $0 < \alpha_{i_0} < \frac{C}{m}$ and there is some $j_0$ such that $0 < \alpha'_{j_0} < \frac{C}{m}$, then by (*) we have $\xi_{i_0} = 0, \xi'_{j_0} = 0$, and we have the two equations
\[
\begin{align*}
    w^\top x_{i_0} - b - y_{i_0} &= \epsilon \\
    -w^\top x_{j_0} + b + y_{j_0} &= \epsilon,
\end{align*}
\]
so $b$ and $\epsilon$ can be computed. In particular,
\[
    b = \frac{1}{2} \left( w^\top (x_{i_0} + x_{j_0}) - (y_{i_0} + y_{j_0}) \right).
\]
The function \( f(x) = w^\top x - b \) (often called regression estimate) is given by

\[
f(x) = \sum_{i=1}^{m} (\alpha'_i - \alpha_i) x_i^\top x_j - b.
\]

The constraints

\[
\sum_{i=1}^{m} (\alpha_i + \alpha'_i) \leq C \nu \\
0 \leq \alpha_i \leq \frac{C}{m} \\
0 \leq \alpha'_i \leq \frac{C}{m}
\]

imply that at most a fraction \( \nu \) of the data can have \( \alpha_i = \frac{C}{m} \) or \( \alpha'_i = \frac{C}{m} \). If follows that if \( \epsilon > 0 \) and \( 0 < \nu \leq 1 \), then \( \nu \) is an upper bound on the fraction of errors.

The KKT conditions imply that if \( \epsilon > 0 \), then \( \beta = 0 \), in which case

\[
\sum_{i=1}^{m} (\alpha_i + \alpha'_i) = C \nu.
\]

Since \( \alpha_i \alpha'_i = 0 \), and since support vectors correspond to \( 0 < \alpha_i, \alpha'_i \leq \frac{C}{m} \), we see that \( \nu \) is a lower bound on the fraction of support vectors.

Since the formulae for \( w, b, \) and \( f(x) \),

\[
w = \sum_{i=1}^{m} (\alpha'_i - \alpha_i) x_i \\
b = \frac{1}{2} \left(w^\top (x_{i_0} + x_{j_0}) - (y_{i_0} + y_{j_0})\right) \\
f(x) = \sum_{i=1}^{m} (\alpha'_i - \alpha_i) x_i^\top x_j - b,
\]

only involve inner products among the data points \( x_i \), and since the objective function \(-G(\alpha, \alpha')\) of the dual program also only involves inner products among the data points \( x_i \), we can kernelize the \( \nu \)-SV regression method.

As in the previous section, we assume that our data points \( \{x_1, \ldots, x_m\} \) belong to a set \( \mathcal{X} \) and we pretend that we have feature space \((F, \langle - , - \rangle)\) and a feature embedding map \( \varphi : \mathcal{X} \rightarrow F \), but we only have access to the kernel function \( \kappa(x_i, x_j) = \langle \varphi(x_i), \varphi(x_j) \rangle \). We wish to perform \( \nu \)-SV regression in the feature space \( F \) on the data set \( \{(\varphi(x_1), y_1), \ldots, (\varphi(x_m), y_m)\} \). Going over the previous computation, we see that the primal program is given by
kernel $\nu$-SV Regression:

$$\text{minimize} \quad \frac{1}{2} \langle w, w \rangle + C \left( \nu \epsilon + \frac{1}{m} \sum_{i=1}^{m} (\xi_i + \xi_i') \right)$$

subject to

$$\langle w, \varphi(x_i) \rangle - b - y_i \leq \epsilon + \xi_i, \quad \xi_i \geq 0 \quad i = 1, \ldots, m$$

$$- \langle w, \varphi(x_i) \rangle + b + y_i \leq \epsilon + \xi_i', \quad \xi_i' \geq 0 \quad i = 1, \ldots, m$$

$$\epsilon \geq 0,$$

minimizing over the variables $w, \epsilon, b, \xi, \xi'$. The Lagrangian is given by

$$L(w, b, \alpha, \alpha', \beta, \xi, \xi', \epsilon, \eta, \eta') = \frac{1}{2} \langle w, w \rangle + \left\langle w, \sum_{i=1}^{m} (\alpha_i - \alpha_i') \varphi(x_i) \right\rangle$$

$$+ \epsilon \left( C\nu - \beta - \sum_{i=1}^{m} (\alpha_i + \alpha_i') \right)$$

$$+ \sum_{i=1}^{m} \xi_i \left( \frac{C}{m} - \alpha_i - \eta_i \right) + \sum_{i=1}^{m} \xi_i' \left( \frac{C}{m} - \alpha_i' - \eta_i' \right)$$

$$- b \left( \sum_{i=1}^{m} (\alpha_i - \alpha_i') \right) - \sum_{i=1}^{m} (\alpha_i - \alpha_i') y_i.$$

Setting the gradient $\nabla L_{w, \epsilon, b, \xi, \xi'}$ of the Lagrangian to zero, we also obtain the equations

$$w = \sum_{i=1}^{m} (\alpha_i' - \alpha_i) \varphi(x_i), \quad (\star_w)$$

$$C\nu - \beta - \sum_{i=1}^{m} (\alpha_i + \alpha_i') = 0$$

$$\sum_{i=1}^{m} (\alpha_i - \alpha_i') = 0$$

$$\frac{C}{m} - \alpha - \eta = 0, \quad \frac{C}{m} - \alpha' - \eta' = 0.$$
minimize \( \frac{1}{2} \sum_{i,j=1}^{m} (\alpha'_i - \alpha_i)(\alpha'_j - \alpha_j)\kappa(x_i, x_j) + \sum_{i=1}^{m} (\alpha_i - \alpha'_i)y_i \)

subject to

\[ \sum_{i=1}^{m} (\alpha_i + \alpha'_i) \leq C\nu \]
\[ \sum_{i=1}^{m} (\alpha_i - \alpha'_i) = 0 \]
\[ 0 \leq \alpha_i \leq \frac{C}{m}, \quad 0 \leq \alpha'_i \leq \frac{C'}{m}, \quad i = 1, \ldots, m. \]

Everything we said before also applies to the kernel \( \nu \)-SV regression method, except that \( x_i \) is replaced by \( \varphi(x_i) \) and that the inner product \( \langle -,- \rangle \) must be used, and we have the formulae

\[ w = \sum_{i=1}^{m} (\alpha'_i - \alpha_i)\varphi(x_i) \]
\[ b = \frac{1}{2} \left( \sum_{i=1}^{m} (\alpha'_i - \alpha_i)\left(\kappa(x_i x_{i0}) + \kappa(x_i, x_{j0})\right) - (y_{i0} + y_{j0}) \right) \]
\[ f(x) = \sum_{i=1}^{m} (\alpha'_i - \alpha_i)\kappa(x_i, x_j) - b, \]

expressions that only involve \( \kappa \).

**Remark:** There is a variant of \( \nu \)-SV regression obtained by setting \( \nu = 0 \) and holding \( \epsilon > 0 \) fixed. This method is called \( \epsilon \)-SV regression or (linear) \( \epsilon \)-insensitive SV regression. The corresponding optimization program is

**\( \epsilon \)-SV Regression:**

\[
\text{minimize} \quad \frac{1}{2} w^\top w + \frac{C}{m} \sum_{i=1}^{m} (\xi_i + \xi'_i)
\]

subject to

\[ w^\top x_i - b - y_i \leq \epsilon + \xi_i, \quad \xi_i \geq 0 \quad i = 1, \ldots, m \]
\[ -w^\top x_i + b + y_i \leq \epsilon + \xi'_i, \quad \xi'_i \geq 0 \quad i = 1, \ldots, m, \]

minimizing over the variables \( w, b, \xi, \) and \( \xi' \).

It is easy to see that the dual program is
minimize \( \frac{1}{2} \sum_{i,j=1}^{m} (\alpha'_i - \alpha_i)(\alpha'_j - \alpha_j)x_i^\top x_j + \sum_{i=1}^{m} (\alpha_i - \alpha'_i)y_i + \epsilon \sum_{i=1}^{m} (\alpha_i + \alpha'_i) \)

subject to
\[
\sum_{i=1}^{m} (\alpha_i - \alpha'_i) = 0
\]
\[
0 \leq \alpha_i \leq \frac{C}{m}, \quad 0 \leq \alpha'_i \leq \frac{C}{m}, \quad i = 1, \ldots, m.
\]

The constraint
\[
\sum_{i=1}^{m} (\alpha_i + \alpha'_i) \leq C\nu
\]
is gone but the extra term \( \epsilon \sum_{i=1}^{m} (\alpha_i + \alpha'_i) \) has been added to the dual function, to prevent \( \alpha_i \) and \( \alpha'_i \) from blowing up.

There is an obvious kernelized version of \( \nu \)-SV regression. It is easy to show that \( \nu \)-SV regression subsumes \( \epsilon \)-SV regression, in the sense that if \( \nu \)-SV regression succeeds and yields \( w, b, \epsilon > 0 \), then \( \epsilon \)-SV regression with the same \( C \) and the same value of \( \epsilon \) also succeeds and returns the same pair \( (w, b) \). For more details on these methods, see Schölkopf, Smola, Williamson, and Bartlett [88].

**Remark:** The linear penalty function \( \sum_{i=1}^{m} (\xi_i + \xi'_i) \) can be repaced by the quadratic penalty function \( \sum_{i=1}^{m} (\xi_i^2 + \xi'_i^2) \); see Shawe-Taylor and Christianini [97] (Chapter 7).

Yet another variant of \( \nu \)-SV regression is to add the term \( \frac{1}{2} b^2 \) to the objective function. The new Lagrangian is
\[
L(w, b, \alpha, \alpha', \beta, \xi, \eta, \xi', \eta') = \frac{1}{2} w^\top w + w^\top \left( \sum_{i=1}^{m} (\alpha_i - \alpha'_i)x_i \right) + \epsilon \left( C\nu - \beta - \sum_{i=1}^{m} (\alpha_i + \alpha'_i) \right) + \sum_{i=1}^{m} \xi_i \left( \frac{C}{m} - \alpha_i - \eta_i \right) + \sum_{i=1}^{m} \xi'_i \left( \frac{C}{m} - \alpha'_i - \eta'_i \right) + \frac{1}{2} b^2 - b \left( \sum_{i=1}^{m} (\alpha_i - \alpha'_i) \right) - \sum_{i=1}^{m} (\alpha_i - \alpha'_i)y_i.
\]

We obtain the new equation
\[
b = \sum_{i=1}^{m} (\alpha_i - \alpha'_i)
determining $b$, which replaces the equation
\[ \sum_{i=1}^{m} (\alpha_i - \alpha'_i) = 0. \]

The new dual program is

\[
\begin{align*}
\text{minimize} & \quad \frac{1}{2} \sum_{i,j=1}^{m} (\alpha'_i - \alpha_i)(\alpha'_j - \alpha_j)(x_i^\top x_j + 1) + \sum_{i=1}^{m} (\alpha_i - \alpha'_i)y_i \\
\text{subject to} & \quad \sum_{i=1}^{m} (\alpha_i + \alpha'_i) \leq C\nu \\
& \quad 0 \leq \alpha_i \leq \frac{C}{m}, \quad 0 \leq \alpha'_i \leq \frac{C}{m}, \quad i = 1, \ldots, m.
\end{align*}
\]
Chapter 17

Soft Margin Support Vector Machines

If the sets of points \( \{ u_1, \ldots, u_p \} \) and \( \{ v_1, \ldots, v_q \} \) are not linearly separable (with \( u_i, v_j \in \mathbb{R}^n \)), we can use a trick from linear programming, which is to introduce nonnegative “slack variables” \( \epsilon = (\epsilon_1, \ldots, \epsilon_p) \in \mathbb{R}^p \) and \( \xi = (\xi_1, \ldots, \xi_q) \in \mathbb{R}^q \) to relax the “hard” constraints
\[
\begin{align*}
    w^\top u_i - b &\geq \delta & i = 1, \ldots, p \\
    -w^\top v_j + b &\geq \delta & j = 1, \ldots, q
\end{align*}
\]
of Problem (SVM\(_{h1}\)) from Section 31.3 to the “soft” constraints
\[
\begin{align*}
    w^\top u_i - b &\geq \delta - \epsilon_i, & \epsilon_i \geq 0 & i = 1, \ldots, p \\
    -w^\top v_j + b &\geq \delta - \xi_j, & \xi_j \geq 0 & j = 1, \ldots, q.
\end{align*}
\]

Recall that \( w \in \mathbb{R}^n \) and \( b, \delta \in \mathbb{R} \).

If \( \epsilon_i > 0 \), the point \( u_i \) may be misclassified, in the sense that it can belong to the margin (the slab), or even to the wrong half-space classifying the negative (red) points. See Figures 34.1 (2) and (3). Similarly, if \( \xi_j > 0 \), the point \( v_j \) may be misclassified, in the sense that it can belong to the margin (the slab), or even to the wrong half-space classifying the positive (blue) points. We can think of \( \epsilon_i \) as a measure of how much the constraint \( w^\top u_i - b \geq \delta \) is violated, and similarly of \( \xi_j \) as a measure of how much the constraint \( -w^\top v_j + b \geq \delta \) is violated. If \( \epsilon = 0 \) and \( \xi = 0 \), then we recover the original constraints. By making \( \epsilon \) and \( \xi \) large enough, these constraints can always be satisfied. We add the constraint \( \delta^\top w \leq 1 \) and we minimize \( -\delta \).

If instead of the constraints of Problem (SVM\(_{h1}\)) we use the hard constraints
\[
\begin{align*}
    w^\top u_i - b &\geq 1 & i = 1, \ldots, p \\
    -w^\top v_j + b &\geq 1 & j = 1, \ldots, q
\end{align*}
\]
of Problem (SVM\(_{h2}\)) (see Example 31.4), then we relax to the soft constraints
\[
\begin{align*}
    w^\top u_i - b &\geq 1 - \epsilon_i, & \epsilon_i \geq 0 & i = 1, \ldots, p \\
    -w^\top v_j + b &\geq 1 - \xi_j, & \xi_j \geq 0 & j = 1, \ldots, q.
\end{align*}
\]
In this case, there is no constraint on \( w \), but we minimize \((1/2)w^\top w\).

Ideally we would like to find a separating hyperplane that minimizes the number of misclassified points, which means that the variables \( \epsilon_i \) and \( \xi_j \) should be as small as possible, but there is a trade-off in maximizing the margin (the thickness of the slab), and minimizing the number of misclassified points. This is reflected in the choice of the objective function, and there are several options, depending on whether we minimize a linear function of the variables \( \epsilon_i \) and \( \xi_j \), or a quadratic functions of these variables, or whether we include the term \((1/2)b^2\) in the objective function. These methods are known as support vector classification algorithms (for short SVC algorithms).

SVC algorithms seek an “optimal” separating hyperplane \( H \) of equation \( w^\top x - b = 0 \). If some new data \( x \in \mathbb{R}^n \) comes in, we can classify it by determining in which of the two half spaces determined by the hyperplane \( H \) they belong, by computing the sign of the quantity \( w^\top x - b \). The function \( \text{sgn}: \mathbb{R} \to \{-1, 1\} \) is given by

\[
\text{sgn}(x) = \begin{cases} 
+1 & \text{if } x \geq 0 \\
-1 & \text{if } x < 0.
\end{cases}
\]

Then we define the (binary) classification function associated with the hyperplane \( H \) of equation \( w^\top x - b = 0 \) as

\[
f(x) = \text{sgn}(w^\top x - b).
\]

Remarkably, all the known optimization problems for finding this hyperplane share the property that the weight vector \( w \) and the constant \( b \) are given by expressions that only involves inner products of the input data points \( u_i \) and \( v_j \), and so does the classification function

\[
f(x) = \text{sgn}(w^\top x - b).
\]

This is a key fact that allows a far reaching generalization of the support vector machine using the method of kernels.

The method of kernels consists in assuming that the input space \( \mathbb{R}^n \) is embedded in a larger (possibly infinite dimensional) Euclidean space \( F \) (with an inner product \( \langle -, - \rangle \)) usually called a feature space, using a function

\[
\varphi: \mathbb{R}^n \to F
\]
called a feature map. The function \( \kappa: \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R} \) given by

\[
\kappa(x, y) = \langle \varphi(x), \varphi(y) \rangle
\]
is the kernel function associated with the embedding \( \varphi \); see Chapter 33. The idea is that the feature map \( \varphi \) “unwinds” the input data, making it somehow more linear in the higher dimensional space \( F \). Now even if we don’t know what the feature space \( F \) is and what the
embedding map \( \varphi \) is, we can pretend to solve our separation problem in \( F \) for the embedded data points \( \varphi(u_i) \) and \( \varphi(v_j) \). Thus we seek a hyperplane \( H \) of equation

\[
\langle w, \zeta \rangle - b = 0, \quad \zeta \in F,
\]

in the feature space \( F \), to attempt to separate the points \( \varphi(u_i) \) and the points \( \varphi(v_j) \). As we said, it turns out that \( w \) and \( b \) are given by expression involving only the inner products

\[
\kappa(u_i, u_j) = \langle \varphi(u_i), \varphi(u_j) \rangle, \quad \kappa(u_i, v_j) = \langle \varphi(u_i), \varphi(v_j) \rangle, \quad \kappa(v_i, v_j) = \langle \varphi(v_i), \varphi(v_j) \rangle,
\]

which form the symmetric \((p + q) \times (p + q)\) matrix \( K \) (a kernel matrix) given by

\[
K_{ij} = \begin{cases}
\kappa(u_i, u_j) & 1 \leq i \leq p, 1 \leq j \leq q \\
-\kappa(u_i, v_{j-p}) & 1 \leq i \leq p, p + 1 \leq j \leq p + q \\
-\kappa(v_{i-p}, u_j) & p + 1 \leq i \leq p + q, 1 \leq j \leq p \\
\kappa(v_{i-p}, v_{j-q}) & p + 1 \leq i \leq p + q, p + 1 \leq j \leq p + q.
\end{cases}
\]

Then the classification function

\[
f(x) = \text{sgn}(\langle w, \varphi(x) \rangle - b)
\]

for points in the original data space \( \mathbb{R}^n \) is also expressed solely in terms of the matrix \( K \) and the inner products \( \kappa(u_i, x) = \langle \varphi(u_i), \varphi(x) \rangle \) and \( \kappa(v_j, x) = \langle \varphi(v_j), \varphi(x) \rangle \). As a consequence, in the original data space \( \mathbb{R}^n \), the hypersurface

\[
S = \{ x \in \mathbb{R}^n \mid \langle w, \varphi(x) \rangle - b = 0 \}
\]

separates the data points \( u_i \) and \( v_j \), but it is not an affine subspace of \( \mathbb{R}^n \). The classification function \( f \) tells us on which “side” of \( S \) is a new data point \( x \in \mathbb{R}^n \). Thus, we managed to separate the data points \( u_i \) and \( v_j \) that are not separable by an affine hyperplane, by a nonaffine hypersurface \( S \), by assuming that an embedding \( \varphi: \mathbb{R}^n \to F \) exists, even though we don’t know what it is, but having access to \( F \) through the kernel function \( \kappa: \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R} \) given by the inner products \( \kappa(x, y) = \langle \varphi(x), \varphi(y) \rangle \).

In practice, the art of using the kernel method is to choose the right kernel (as the knight says in Indiana Jones, to “choose wisely.”).

The method of kernels is very flexible. It also applies to the soft margin versions of SVM, but also to regression problems, and to principal component analysis (PCA), and to other problems arising in machine learning.

Comprehensive presentations of the method of kernels are found in Schölkopf and Smola [86] and Shawe–Taylor and Christianini [97]. See also Bishop [18].

We first consider the soft margin SVM arising from Problem (SVM_{h1}).
CHAPTER 17. SOFT MARGIN SUPPORT VECTOR MACHINES

17.1 Soft Margin Support Vector Machines; \((\text{SVM}_{s1})\)

In this section we derive the dual function \(G\) associated with the following version of the soft margin SVM coming from Problem \((\text{SVM}_{h1})\), where the maximization of the margin \(\delta\) has been replaced by the minimization of \(-\delta\), and where we added a “regularizing term” \(K \left( \sum_{i=1}^{p} \epsilon_i + \sum_{j=1}^{q} \xi_j \right)\) whose purpose is to make \(\epsilon \in \mathbb{R}^p\) and \(\xi \in \mathbb{R}^q\) sparse (that is, try to make \(\epsilon_i\) and \(\xi_j\) have as many zeros as possible), where \(K > 0\) is a fixed constant that can be adjusted to determine the influence of this regularizing term. If the primal problem \((\text{SVM}_{s1})\) has an optimal solution \((w, \delta, b, \epsilon, \xi)\), we attempt to use the dual function \(G\) to obtain it, but we will see that with this particular formulation of the problem, the constraint \(w^\top w \leq 1\) causes troubles, even though it is convex.

**Soft margin SVM \((\text{SVM}_{s1})\):**

\[
\begin{align*}
\text{minimize} & \quad -\delta + K \left( \sum_{i=1}^{p} \epsilon_i + \sum_{j=1}^{q} \xi_j \right) \\
\text{subject to} & \quad w^\top u_i - b \geq \delta - \epsilon_i, \quad \epsilon_i \geq 0 \quad i = 1, \ldots, p \\
& \quad -w^\top v_j + b \geq \delta - \xi_j, \quad \xi_j \geq 0 \quad j = 1, \ldots, q \\
& \quad w^\top w \leq 1.
\end{align*}
\]

It is customary to write \(\ell = p + q\).

For this problem, the primal problem may have an optimal solution \((w, \delta, b, \epsilon, \xi)\) with \(\|w\| = 1\) and \(\delta > 0\), but if the sets of points are not linearly separable then an optimal solution of the dual may not yield \(w\).

The objective function of our problem is affine and the only nonaffine constraint \(w^\top w \leq 1\) is convex. This constraint is qualified because for any \(w \neq 0\) such that \(w^\top w < 1\) and for any \(\delta > 0\) and any \(b\) we can pick \(\epsilon\) and \(\xi\) large enough so that the constraints are satisfied. Consequently, by Theorem 31.14(2) if the primal problem \((\text{SVM}_{s1})\) has an optimal solution, then the dual problem has a solution too, and the duality gap is zero.

Unfortunately this does not imply that an optimal solution of the dual yields an optimal solution of the primal because the hypotheses of Theorem 31.14(1) fail to hold. In general, there may not be a unique vector \((w, \epsilon, \xi, b, \delta)\) such that

\[
\inf_{w, \epsilon, \xi, b, \delta} L(w, \epsilon, \xi, b, \delta, \lambda, \alpha, \beta, \gamma) = G(\lambda, \mu, \alpha, \beta, \gamma).
\]

If the sets \(\{u_i\}\) and \(\{v_j\}\) are not linearly separable, then the dual problem may have a solution for which \(\gamma = 0\),

\[
\sum_{i=1}^{p} \lambda_i = \sum_{j=1}^{q} \mu_j = \frac{1}{2}.
\]
and
\[ \sum_{i=1}^{p} \lambda_i u_i = \sum_{j=1}^{q} \mu_j v_j, \]
so that the dual function \( G(\lambda, \mu, \alpha, \beta, \gamma) \), which is a partial function, is defined and has the value \( G(\lambda, \mu, \alpha, \beta, 0) = 0 \). Such a pair \((\lambda, \mu)\) corresponds to the coefficients of two convex combinations
\[ \sum_{i=1}^{p} 2\lambda_i u_i = \sum_{j=1}^{q} 2\mu_j v_j, \]
which correspond to the same point in the (nonempty) intersection of the convex hulls \( \text{conv}(u_1, \ldots, u_p) \) and \( \text{conv}(v_1, \ldots, v_q) \). It turns out that the only connection between \( w \) and the dual function is the equation
\[ 2\gamma w = \sum_{i=1}^{p} \lambda_i u_i - \sum_{j=1}^{q} \mu_j v_j, \]
and when \( \gamma = 0 \) this is equation is \( 0 = 0 \), so the dual problem is useless to determine \( w \). This point seems to have been missed in the literature (for example, in Shawe–Taylor and Christianini [97], Section 7.2). What the dual problem does show is that \( \delta \geq 0 \). However, if \( \gamma \neq 0 \), then \( w \) is determined by any solution \((\lambda, \mu)\) of the dual.

It still remains to compute \( \delta \) and \( b \), which can be done under a mild hypothesis that we call the Standard Margin Hypothesis.

If \((w, \delta, b, \epsilon, \xi)\) is an optimal solution of Problem \((\text{SVM}_{s_1})\), then the points \( u_i \) and \( v_j \) are classified as follows:

1. If \( \epsilon_i = 0 \), then the point \( u_i \) is correctly classified and is either on the blue margin (the hyperplane \( H_{w, b+\eta} \) of equation \( w^\top x = b + \eta \)) or on the correct side of the blue margin (the blue side). Similarly, if \( \xi_j = 0 \), then the point \( v_j \) is correctly classified and is either on the red margin (the hyperplane \( H_{w, b-\eta} \) of equation \( w^\top x = b - \eta \)) or on the correct side of the red margin (the red side).

2. If \( 0 < \epsilon_i \leq \eta \), then the point \( u_i \) lies inside the margin (the slab), but on the correct side of the separating hyperplane (the blue side). If \( \epsilon_i = \eta \), then \( u_i \) lies on the separating hyperplane. Similarly, if \( 0 < \xi_j \leq \eta \), then the point \( v_j \) lies inside the margin (the slab), but on the correct side of the separating hyperplane (the red side). If \( \xi_j = \eta \), then \( v_j \) lies on the separating hyperplane.

3. If \( \epsilon_i > \eta \), then the point \( u_i \) lies on the wrong side of the separating hyperplane (the red side); it is misclassified. Similarly, if \( \xi_j > \eta \), then the point \( v_j \) lies on the wrong side of the separating hyperplane (the blue side); it is misclassified.
Let \( \lambda \in \mathbb{R}_+^p \) be the Lagrange multipliers associated with the inequalities \( w^\top u_i - b \geq \delta - \epsilon_i \), let \( \mu \in \mathbb{R}_+^q \) be the Lagrange multipliers associated with the inequalities \( -w^\top v_j + b \geq \delta - \xi_j \), let \( \alpha \in \mathbb{R}_+^p \) be the Lagrange multipliers associated with the inequalities \( \epsilon_i \geq 0 \), \( \beta \in \mathbb{R}_+^q \) be the Lagrange multipliers associated with the inequalities \( \xi_j \geq 0 \), and let \( \gamma \in \mathbb{R}_+ \) be the Lagrange multiplier associated with the inequality \( w^\top w \leq 1 \).

The linear constraints are given by the \( 2(p + q) \times (n + p + q + 2) \) matrix given in block form by

\[
C = \begin{pmatrix}
X^\top & -I_{p+q} & 1_p & 1_{p+q} \\
0_{p+q,n} & -I_{p+q} & 0_{p+q} & 0_{p+q}
\end{pmatrix},
\]

where \( X \) is the \( n \times (p + q) \) matrix

\[
X = (-u_1 \cdots -u_p \ v_1 \cdots v_q),
\]

and the linear constraints are expressed by

\[
\begin{pmatrix}
X^\top & -I_{p+q} & 1_p & 1_{p+q} \\
0_{p+q,n} & -I_{p+q} & 0_{p+q} & 0_{p+q}
\end{pmatrix}
\begin{pmatrix}
w \\
\epsilon \\
\xi \\
\beta
\end{pmatrix}
\leq
\begin{pmatrix}
0_{p+q} \\
0_{p+q}
\end{pmatrix}.
\]

More explicitly, \( C \) is the following matrix:

\[
C = \begin{pmatrix}
-u_1^\top & -1 & \cdots & 0 & 0 & \cdots & 0 & 1 & 1 \\
\vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
-u_p^\top & 0 & \cdots & -1 & 0 & \cdots & 0 & 1 & 1 \\
0 & 0 & \cdots & 0 & -1 & \cdots & 0 & -1 & 1 \\
\vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
0 & 0 & \cdots & 0 & 0 & \cdots & -1 & -1 & 1 \\
0 & -1 & \cdots & 0 & 0 & \cdots & 0 & 0 & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
0 & 0 & \cdots & -1 & 0 & \cdots & 0 & 0 & 0 \\
0 & 0 & \cdots & 0 & -1 & \cdots & 0 & 0 & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
0 & 0 & \cdots & 0 & 0 & \cdots & -1 & 0 & 0 \\
0 & 0 & \cdots & 0 & 0 & \cdots & 0 & 0 & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
\vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
0 & 0 & \cdots & 0 & 0 & \cdots & -1 & 0 & 0
\end{pmatrix}.
\]

The objective function is given by

\[
J(w, \epsilon, \xi, b, \delta) = -\delta + K(\epsilon^\top \xi^\top)1_{p+q}.
\]
The Lagrangian $L(w, \epsilon, \xi, b, \delta, \lambda, \mu, \alpha, \beta, \gamma)$ with $\lambda, \alpha \in \mathbb{R}^p_+, \mu, \beta \in \mathbb{R}^q_+$, and $\gamma \in \mathbb{R}^+$ is given by

$$L(w, \epsilon, \xi, b, \delta, \lambda, \mu, \alpha, \beta, \gamma) = -\delta + K(\epsilon^\top \xi^\top) \mathbf{1}_{p+q} + (w^\top (\epsilon^\top \xi^\top) b \delta) C^\top \begin{pmatrix} \lambda \\ \mu \\ \alpha \\ \beta \end{pmatrix} + \gamma(w^\top w - 1).$$

Since

$$\begin{pmatrix} w^\top (\epsilon^\top \xi^\top) b \delta \end{pmatrix} C^\top \begin{pmatrix} \lambda \\ \mu \\ \alpha \\ \beta \end{pmatrix} = w^\top X \begin{pmatrix} \lambda \\ \mu \\ \alpha \\ \beta \end{pmatrix} - \epsilon^\top (\lambda + \alpha) - \xi^\top (\mu + \beta) + b(1_p^\top \lambda - 1_q^\top \mu) + \delta(1_p^\top \lambda + 1_q^\top \mu),$$

the Lagrangian can be written as

$$L(w, \epsilon, \xi, b, \delta, \lambda, \mu, \alpha, \beta, \gamma) = -\delta + K(\epsilon^\top \mathbf{1}_p + \xi^\top \mathbf{1}_q) + w^\top X \begin{pmatrix} \lambda \\ \mu \\ \alpha \\ \beta \end{pmatrix} + \gamma(w^\top w - 1) - \epsilon^\top (\lambda + \alpha) - \xi^\top (\mu + \beta) + b(1_p^\top \lambda - 1_q^\top \mu) + \delta(1_p^\top \lambda + 1_q^\top \mu) = (1_p^\top \lambda + 1_q^\top \mu - 1)\delta + w^\top X \begin{pmatrix} \lambda \\ \mu \\ \alpha \\ \beta \end{pmatrix} + \gamma(w^\top w - 1) + \epsilon^\top (K1_p - (\lambda + \alpha)) + \xi^\top (K1_q - (\mu + \beta)) + b(1_p^\top \lambda - 1_q^\top \mu).$$

To find the dual function $G(\lambda, \mu, \alpha, \beta, \gamma)$ we minimize $L(w, \epsilon, \xi, b, \delta, \lambda, \mu, \alpha, \beta, \gamma)$ with respect to $w, \epsilon, \xi, b, \delta$. Since the Lagrangian is convex and $(w, \epsilon, \xi, b, \delta) \in \mathbb{R}^n \times \mathbb{R}^p \times \mathbb{R}^q \times \mathbb{R} \times \mathbb{R}$, a convex open set, by Theorem 21.11, the Lagrangian has a minimum in $(w, \epsilon, \xi, b, \delta)$ iff $\nabla L_{w, \epsilon, \xi, b, \delta} = 0$, so we compute the gradient with respect to $w, \epsilon, \xi, b, \delta$ and we get

$$\nabla L_{w, \epsilon, \xi, b, \delta} = \begin{pmatrix} X \begin{pmatrix} \lambda \\ \mu \end{pmatrix} + 2\gamma w \\ K1_p - (\lambda + \alpha) \\ K1_q - (\mu + \beta) \\ 1_p^\top \lambda - 1_q^\top \mu \\ 1_p^\top \lambda + 1_q^\top \mu - 1 \end{pmatrix}. $$

By setting $\nabla L_{w, \epsilon, \xi, b, \delta} = 0$ we get the equations

$$2\gamma w = -X \begin{pmatrix} \lambda \\ \mu \end{pmatrix} \quad (\ast_w)$$
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and

\[
\begin{align*}
\lambda + \alpha &= K1_p \\
\mu + \beta &= K1_q \\
1_p^\top \lambda &= 1_q^\top \mu \\
1_p^\top \lambda + 1_q^\top \mu &= 1.
\end{align*}
\]

The second and third equations are equivalent to the inequalities

\[
0 \leq \lambda_i, \mu_j \leq K, \quad i = 1, \ldots, p, \quad j = 1, \ldots, q,
\]

often called box constraints, and the fourth and fifth equations yield

\[
1_p^\top \lambda = 1_q^\top \mu = \frac{1}{2}.
\]

First let us consider the singular case \(\gamma = 0\). In this case, \((\ast_w)\) implies that

\[
X \begin{pmatrix} \lambda \\ \mu \end{pmatrix} = 0,
\]

and the term \(\gamma(w^\top w - 1)\) is missing from the Lagrangian, which in view of the other four equations above reduces to

\[
L(w, \epsilon, \xi, b, \delta, \lambda, \mu, \alpha, \beta, 0) = w^\top X \begin{pmatrix} \lambda \\ \mu \end{pmatrix} = 0.
\]

In summary, we proved that if \(\gamma = 0\), then

\[
G(\lambda, \mu, \alpha, \beta, 0) = \begin{cases} 
0 & \text{if } \begin{cases} 
\sum_{i=1}^p \lambda_i = \sum_{j=1}^q \mu_j = \frac{1}{2} \\
0 \leq \lambda_i \leq K, \ i = 1, \ldots, p \\
0 \leq \mu_j \leq K, \ j = 1, \ldots, q \\
\text{and } \sum_{i=1}^p \lambda_i u_i - \sum_{j=1}^q \mu_j v_j = 0.
\end{cases} \\
-\infty & \text{otherwise}
\end{cases}
\]

Geometrically, \((\lambda, \mu)\) corresponds to the coefficients of two convex combinations

\[
\sum_{i=1}^p 2\lambda_i u_i = \sum_{j=1}^q 2\mu_j v_j
\]

which correspond to the same point in the intersection of the convex hulls \(\text{conv}(u_1, \ldots, u_p)\) and \(\text{conv}(v_1, \ldots, v_q)\), iff the sets \(\{u_i\}\) and \(\{v_j\}\) are not linearly separable. If the sets \(\{u_i\}\) and \(\{v_j\}\) are linearly separable, then the convex hulls \(\text{conv}(u_1, \ldots, u_p)\) and \(\text{conv}(v_1, \ldots, v_q)\) are disjoint, which implies that \(\gamma > 0\).
Let us now assume that $\gamma > 0$. Plugging back $w$ from equation (*w,) into the Lagrangian, after simplifications we get

$$G(\lambda, \mu, \alpha, \beta, \gamma) = -\frac{1}{2\gamma} (\lambda^\top \mu^\top) X^\top X \left(\begin{array}{c} \lambda \\ \mu \end{array}\right) + \frac{\gamma}{4\gamma^2} (\lambda^\top \mu^\top) X^\top X \left(\begin{array}{c} \lambda \\ \mu \end{array}\right) - \gamma$$

$$= -\frac{1}{4\gamma} (\lambda^\top \mu^\top) X^\top X \left(\begin{array}{c} \lambda \\ \mu \end{array}\right) - \gamma,$$

so if $\gamma > 0$ the dual function is independent of $\alpha, \beta$ and is given by

$$G(\lambda, \mu, \alpha, \beta, \gamma) = \begin{cases} -\frac{1}{4\gamma} (\lambda^\top \mu^\top) X^\top X \left(\begin{array}{c} \lambda \\ \mu \end{array}\right) - \gamma & \text{if } \gamma > 0 \\ -\infty & \text{otherwise.} \end{cases}$$

Since $X^\top X$ is symmetric positive definite and $\gamma \geq 0$, obviously

$$G(\lambda, \mu, \alpha, \beta, \gamma) \leq 0$$

for all $\gamma > 0$.

The dual program is given by

maximize $-\frac{1}{4\gamma} (\lambda^\top \mu^\top) X^\top X \left(\begin{array}{c} \lambda \\ \mu \end{array}\right) - \gamma$ if $\gamma > 0$

subject to

$$\sum_{i=1}^p \lambda_i = \sum_{j=1}^q \mu_j = \frac{1}{2}$$

$$0 \leq \lambda_i \leq K, \quad i = 1, \ldots, p$$

$$0 \leq \mu_j \leq K, \quad j = 1, \ldots, q.$$

Also, if $\gamma = 0$ then $X \left(\begin{array}{c} \lambda \\ \mu \end{array}\right) = 0$.

Maximizing with respect to $\gamma > 0$ yields

$$\gamma^2 = \frac{1}{4} (\lambda^\top \mu^\top) X^\top X \left(\begin{array}{c} \lambda \\ \mu \end{array}\right),$$

so we obtain

$$G(\lambda, \mu) = -\left((\lambda^\top \mu^\top) X^\top X \left(\begin{array}{c} \lambda \\ \mu \end{array}\right)\right)^{1/2}.$$
Finally, since $G(\lambda, \mu) = 0$ and $X \begin{pmatrix} \lambda \\ \mu \end{pmatrix} = 0$ if $\gamma = 0$, the dual program is equivalent to the following minimization program:

\[
\text{minimize } \begin{pmatrix} \lambda^T \\ \mu^T \end{pmatrix} X^T X \begin{pmatrix} \lambda \\ \mu \end{pmatrix}
\]

subject to

\[
\sum_{i=1}^{p} \lambda_i = \sum_{j=1}^{q} \mu_j = \frac{1}{2},
\]
\[
0 \leq \lambda_i \leq K, \quad i = 1, \ldots, p,
\]
\[
0 \leq \mu_j \leq K, \quad j = 1, \ldots, q.
\]

Observe that the constraints imply that $K$ must be chosen so that

\[
K \geq \max \left\{ \frac{1}{2p}, \frac{1}{2q} \right\}.
\]

The dual program is solved by making use of numerical procedures based on gradient descent. If the primal problem is solvable, this yields solutions for $\lambda$ and $\mu$.

If the optimal value is 0, then $\gamma = 0$ and $X \begin{pmatrix} \lambda \\ \mu \end{pmatrix} = 0$, so in this case it is not possible to determine $w$. However, if the optimal value is $> 0$, then once a solution for $\lambda$ and $\mu$ is obtained, by $(\ast_w)$, we have

\[
\gamma = \frac{1}{2} \left( \begin{pmatrix} \lambda^T \\ \mu^T \end{pmatrix} X^T X \begin{pmatrix} \lambda \\ \mu \end{pmatrix} \right)^{1/2},
\]
\[
w = \frac{1}{2\gamma} \left( \sum_{i=1}^{p} \lambda_i u_i - \sum_{j=1}^{q} \mu_j v_j \right),
\]

so we get

\[
w = \frac{\sum_{i=1}^{p} \lambda_i u_i - \sum_{j=1}^{q} \mu_j v_j}{\left( \begin{pmatrix} \lambda^T \\ \mu^T \end{pmatrix} X^T X \begin{pmatrix} \lambda \\ \mu \end{pmatrix} \right)^{1/2}},
\]

which is the result of making $\sum_{i=1}^{p} \lambda_i u_i - \sum_{j=1}^{q} \mu_j v_j$ a unit vector, since

\[
X = (-u_1 \cdots -u_p \ v_1 \cdots v_q).
\]

It remains to find $b$ and $\delta$, which are not given by the dual program.
The complementary slackness conditions yield a classification of the points in terms of the values of $\lambda$ and $\mu$. Indeed, we have $\epsilon_i\alpha_i = 0$ for $i = 1, \ldots, p$ and $\xi_j\beta_j = 0$ for $j = 1, \ldots, q$.

Also, if $\lambda_i > 0$, then corresponding constraint is active, and similarly if $\mu_j > 0$. Since $\lambda_i + \alpha_i = K$, it follows that $\epsilon_i\alpha_i = 0$ iff $\epsilon_i(K - \lambda_i) = 0$, and since $\mu_j + \beta_j = K$, we have $\xi_j\beta_j = 0$ iff $\xi_j(K - \mu_j) = 0$. Thus if $\epsilon_i > 0$ then $\lambda_i = K$, and if $\xi_j > 0$, then $\mu_j = K$. Consequently, if $\lambda_i < K$ then $\epsilon_i = 0$ and $u_i$ is correctly classified, and similarly if $\mu_j < K$ then $\xi_j = 0$ and $v_j$ is correctly classified. We have the following classification:

1. If $0 < \lambda_i < K$ then $u_i$ is on the margin and is classified correctly. Similarly, if $0 < \mu_j < K$ then $v_j$ is on the margin and is classified correctly.

2. If $\lambda_i = K$, then if $\epsilon_i \leq \delta$ the point $u_i$ may be classified correctly or it lies within the margin on the correct side, but if $\epsilon_i > \delta$ then it is misclassified. Similarly, if $\mu_j = K$, then if $\xi_j \leq \delta$ the point $v_j$ may be classified correctly or it lies within the margin on the correct side, but if $\xi_j > \delta$ then it is misclassified.

3. If $\lambda_i = 0$ then $u_i$ is classified correctly. Similarly, if $\mu_j = 0$ then $v_j$ is classified correctly.

The equations

$$\sum_{i=1}^{p} \lambda_i = \sum_{j=1}^{q} \mu_j = \frac{1}{2}$$

imply that there is some $i_0$ such that $\lambda_{i_0} > 0$ and some $j_0$ such that $\mu_{j_0} > 0$, but a priori, nothing prevents the situation where $\lambda_i = K$ for all nonzero $\lambda_i$ or $\mu_j = K$ for all nonzero $\mu_j$. If this happens, we can rerun the optimization method with a larger value of $K$. If the following mild hypothesis holds then $b$ and $\delta$ can be found.

**Standard Margin Hypothesis** for $(\text{SVM}_{s_1})$. There is some index $i_0$ such that $0 < \lambda_{i_0} < K$ and there is some index $j_0$ such that $0 < \mu_{j_0} < K$. This means that some $u_{i_0}$ is correctly classified and on the blue margin, and some $v_{j_0}$ is correctly classified and on the red margin.

If the **Standard Margin Hypothesis** for $(\text{SVM}_{s_1})$ holds then $\epsilon_{i_0} = 0$ and $\mu_{j_0} = 0$, and then we have the active equations

$$w^T u_{i_0} - b = \delta \quad \text{and} \quad -w^T v_{j_0} + b = \delta,$$

and we obtain the value of $b$ and $\delta$ as

$$b = \frac{1}{2}(w^T u_{i_0} + w^T v_{j_0})$$

$$\delta = \frac{1}{2}(w^T u_{i_0} - w^T v_{j_0}).$$

As we said earlier, the hypotheses of Theorem 31.14(2) hold, so if the primal problem $(\text{SVM}_{s_1})$ has an optimal solution with $w \neq 0$, then the dual problem has a solution too, and the duality gap is zero. Therefore, for optimal solutions we have

$$L(w, \epsilon, \xi, b, \delta, \lambda, \mu, \alpha, \beta, \gamma) = G(\lambda, \mu, \alpha, \beta, \gamma),$$
which means that

\[-\delta + K \left( \sum_{i=1}^{p} \epsilon_i + \sum_{j=1}^{q} \xi_j \right) = -\left( (\lambda^\top \mu^\top) X^\top X \begin{pmatrix} \lambda \\ \mu \end{pmatrix} \right)^{1/2},\]

so we get

\[\delta = K \left( \sum_{i=1}^{p} \epsilon_i + \sum_{j=1}^{q} \xi_j \right) + \left( (\lambda^\top \mu^\top) X^\top X \begin{pmatrix} \lambda \\ \mu \end{pmatrix} \right)^{1/2}.\]

Therefore, we confirm that \(\delta \geq 0\).

It is important to note that the objective function of the dual program

\[-G(\lambda, \mu) = \left( (\lambda^\top \mu^\top) X^\top X \begin{pmatrix} \lambda \\ \mu \end{pmatrix} \right)^{1/2}\]

only involves the inner products of the \(u_i\) and the \(v_j\) through the matrix \(X^\top X\), and similarly, the equation of the optimal hyperplane can be written as

\[\sum_{i=1}^{p} \lambda_i u_i^\top x - \sum_{j=1}^{q} \mu_j v_j^\top x - (\lambda^\top \mu^\top) X^\top X \begin{pmatrix} \lambda \\ \mu \end{pmatrix}^{1/2} b = 0,\]

an expression that only involves inner products of \(x\) with the \(u_i\) and the \(v_j\) and inner products of the \(u_i\) and the \(v_j\).

As explained at the beginning of this chapter, this is a key fact that allows a generalization of the support vector machine using the method of kernels. We can define the following “kernelized” version of Problem (SVMs1):

**Soft margin kernel SVM (SVMs1):**

\[
\begin{align*}
\text{minimize} & \quad -\delta + K \left( \sum_{i=1}^{p} \epsilon_i + \sum_{j=1}^{q} \xi_j \right) \\
\text{subject to} & \quad \langle w, \varphi(u_i) \rangle - b \geq \delta - \epsilon_i, \quad \epsilon_i \geq 0 \quad i = 1, \ldots, p \\
& \quad -\langle w, \varphi(v_j) \rangle + b \geq \delta - \xi_j, \quad \xi_j \geq 0 \quad j = 1, \ldots, q \\
& \quad \langle w, w \rangle \leq 1.
\end{align*}
\]

Tracing through the computation that led us to the dual program with \(u_i\) replaced by \(\varphi(u_i)\) and \(v_j\) replaced by \(\varphi(v_j)\), we find the following version of the dual program:
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minimize \((\lambda^\top \mu^\top) K \begin{pmatrix} \lambda \\ \mu \end{pmatrix}\)

subject to

\[
\sum_{i=1}^{p} \lambda_i = \sum_{j=1}^{q} \mu_j = \frac{1}{2}
\]

\[
0 \leq \lambda_i \leq K, \quad i = 1, \ldots, p
\]

\[
0 \leq \mu_j \leq K, \quad j = 1, \ldots, q,
\]

where \(K\) is the \(\ell \times \ell\) kernel symmetric matrix (with \(\ell = p + q\)) given by

\[
K_{ij} = \begin{cases} 
\kappa(u_i, u_j) & 1 \leq i \leq p, 1 \leq j \leq q \\
-\kappa(u_i, v_{j-p}) & 1 \leq i \leq p, p + 1 \leq j \leq p + q \\
-\kappa(v_{i-p}, u_j) & p + 1 \leq i \leq p + q, 1 \leq j \leq p \\
\kappa(v_{i-p}, v_{j-q}) & p + 1 \leq i \leq p + q, p + 1 \leq j \leq p + q.
\end{cases}
\]

We also find that

\[
w = \frac{\sum_{i=1}^{p} \lambda_i \varphi(u_i) - \sum_{j=1}^{q} \mu_j \varphi(v_j)}{\left((\lambda^\top \mu^\top) K \begin{pmatrix} \lambda \\ \mu \end{pmatrix}\right)^{1/2}}.
\]

Under the Standard Margin Hypothesis, there is some index \(i_0\) such that \(0 < \lambda_{i_0} < K\) and there is some index \(j_0\) such that \(0 < \mu_{j_0} < K\), and we obtain the value of \(b\) and \(\delta\) as

\[
b = \frac{1}{2}(\langle w, \varphi(u_{i_0}) \rangle + \langle w, \varphi(v_{j_0}) \rangle)
\]

\[
\delta = \frac{1}{2}(\langle w, \varphi(u_{i_0}) \rangle - \langle w, \varphi(v_{j_0}) \rangle).
\]

Using the above value for \(w\), we obtain

\[
b = \frac{\sum_{i=1}^{p} \lambda_i (\kappa(u_i, u_{i_0}) + \kappa(u_i, v_{j_0})) - \sum_{j=1}^{q} \mu_j (\kappa(v_j, u_{i_0}) + \kappa(v_j, v_{j_0}))}{2 \left((\lambda^\top \mu^\top) K \begin{pmatrix} \lambda \\ \mu \end{pmatrix}\right)^{1/2}}.
\]

It follows that the classification function

\[
f(x) = \text{sgn}(\langle w, \varphi(x) \rangle - b)
\]
is given by
\[
f(x) = \text{sgn} \left( \sum_{i=1}^{p} \lambda_i (2\kappa(u_i, x) - \kappa(u_i, u_{i_0}) - \kappa(u_i, v_{j_0})) - \sum_{j=1}^{q} \mu_j (2\kappa(v_j, x) - \kappa(v_j, u_{i_0}) - \kappa(v_j, v_{j_0})) \right),
\]
which is solely expressed in terms of the kernel \( \kappa \).

Kernel methods for SVM are discussed in Schölkopf and Smola [86] and Shawe–Taylor and Christianini [97].

Since the constraint \( w^\top w \leq 1 \) causes troubles, we trade it for a different objective function in which \(-\delta\) is replaced by \((1/2) \|w\|^2\). This way we are left with purely affine constraints. In the next section we discuss a generalization of Problem (SVM_{h2}) obtained by adding a linear regularizing term.

### 17.2 Soft Margin Support Vector Machines; (SVM_{s2})

In this section we consider the generalization of Problem (SVM_{h2}) where we minimize \((1/2)w^\top w\) by adding the “regularizing term” \( K\left( \sum_{i=1}^{p} \epsilon_i + \sum_{j=1}^{q} \xi_j \right) \) for some \( K > 0 \). Recall that the margin \( \delta \) is given by \( \delta = 1/\|w\| \).

**Soft margin SVM (SVM_{s2}):**

\[
\begin{aligned}
\text{minimize} & \quad \frac{1}{2} w^\top w + K \left( \epsilon^\top \xi^\top \right) 1_{p+q} \\
\text{subject to} & \quad w^\top u_i - b \geq 1 - \epsilon_i, \quad \epsilon_i \geq 0 \quad i = 1, \ldots, p \\
& \quad -w^\top v_j + b \geq 1 - \xi_j, \quad \xi_j \geq 0 \quad j = 1, \ldots, q.
\end{aligned}
\]

This is the classical problem discussed in all books on machine learning or pattern analysis, for instance Vapnik [111], Bishop [18], and Shawe–Taylor and Christianini [97]. The trivial solution where all variables are 0 is ruled out because of the presence of the 1 in the inequalities, but it is not clear that if \((w, \epsilon, \xi, b)\) is an optimal solution, then \( w \neq 0 \).

We prove that if the primal problem has an optimal solution \((w, \epsilon, \xi, b)\) with \( w \neq 0 \), then \( w \) is determined by any optimal solution \((\lambda, \mu)\) of the dual. We also prove that there is some \( i \) for which \( \lambda_i > 0 \) and some \( j \) for which \( \mu_j > 0 \). Under a mild hypothesis that we call the **Standard Margin Hypothesis**, \( b \) can be found.

If \((w, \epsilon, \xi, b)\) is an optimal solution of Problem (SVM_{s2}), then the points \( u_i \) and \( v_j \) are classified as follows:
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(1) If \( \epsilon_i = 0 \), then the point \( u_i \) is correctly classified and is either on the margin or on the correct side of the margin (the blue side). Similarly, if \( \xi_j = 0 \), then the point \( v_j \) is correctly classified and is either on the margin or on the correct side of the margin (the red side). See Figure 34.1 (1).

(2) If \( 0 < \epsilon_i \leq 1 \), then the point \( u_i \) lies inside the margin (the slab), but on the correct side of the separating hyperplane \( w^\top x - b = 0 \); this occurs when \( 0 < \epsilon_1 < 1 \). The right illustration depicts \( u_i \) on the separating hyperplane whenever \( \epsilon_1 = 1 \). Figure (3) illustrates a misclassification of \( u_i \) and occurs when \( \epsilon_1 > 1 \).

Points for which \( \epsilon_i > 0 \) (or \( \xi_j > 0 \)) are called margin-errors; they either lie within the slab or they are misclassified.
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Note that this framework is still somewhat sensitive to outliers because the penalty for misclassification is linear in \( \epsilon \) and \( \xi \).

First we write the constraints in matrix form. The \( 2(p + q) \times (n + p + q + 1) \) matrix \( C \) is written in block form as
\[
C = \begin{pmatrix}
X^\top & -I_{p+q} & 1_p \\
0_{p+q,n} & -I_{p+q} & 0_{p+q}
\end{pmatrix},
\]
and the constraints are expressed by
\[
\begin{pmatrix}
X^\top & -I_{p+q} & 1_p \\
0_{p+q,n} & -I_{p+q} & 0_{p+q}
\end{pmatrix}
\begin{pmatrix}
w \\
\epsilon \\
\xi \\
b
\end{pmatrix}
\leq
\begin{pmatrix}
-1_{p+q} \\
0_{p+q}
\end{pmatrix}.
\]

The objective function \( J(w, \epsilon, \xi, b) \) is given by
\[
J(w, \epsilon, \xi, b) = \frac{1}{2} w^\top w + K(\epsilon^\top \xi^\top) 1_{p+q}.
\]

The Lagrangian \( L(w, \epsilon, \xi, b, \lambda, \alpha, \beta) \) with \( \lambda, \alpha \in \mathbb{R}_+^p \) and with \( \mu, \beta \in \mathbb{R}_+^q \) is given by
\[
L(w, \epsilon, \xi, b, \lambda, \alpha, \beta) = \frac{1}{2} w^\top w + K(\epsilon^\top \xi^\top) 1_{p+q}
+ (w^\top (\epsilon^\top \xi^\top) b) C^\top \begin{pmatrix}
\lambda \\
\mu \\
\alpha \\
\beta
\end{pmatrix}
+ (1_{p+q}^\top 0_{p+q}^\top) \begin{pmatrix}
\lambda \\
\mu \\
\alpha \\
\beta
\end{pmatrix}.
\]

Since
\[
(w^\top (\epsilon^\top \xi^\top) b) C^\top \begin{pmatrix}
\lambda \\
\mu \\
\alpha \\
\beta
\end{pmatrix} = (w^\top (\epsilon^\top \xi^\top) b) \begin{pmatrix}
X \\
-1_{p+q}^\top \\
-1_{p+q}^\top
\end{pmatrix}
\begin{pmatrix}
\lambda \\
\mu \\
\alpha \\
\beta
\end{pmatrix}
\]
we get
\[
(w^\top (\epsilon^\top \xi^\top) b) C^\top \begin{pmatrix}
\lambda \\
\mu \\
\alpha \\
\beta
\end{pmatrix} = w^\top X(\lambda) - \epsilon^\top (\lambda + \alpha) - \xi^\top (\mu + \beta) + b(1_p^\top \lambda - 1_q^\top \mu),
\]
where
\[
X(\lambda) = \begin{pmatrix}
\lambda \\
\mu \\
\alpha \\
\beta
\end{pmatrix}.
\]
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and since

\[
\begin{pmatrix}
1^T_{p+q} & 0^T_{p+q}
\end{pmatrix}
\begin{pmatrix}
\lambda \\
\mu \\
\alpha \\
\beta
\end{pmatrix} = 1^T_{p+q} \begin{pmatrix}
\lambda \\
\mu
\end{pmatrix} = (\lambda^T \mu^T) 1_{p+q},
\]

the Lagrangian can be rewritten as

\[
L(w, \epsilon, \xi, b, \lambda, \mu, \alpha, \beta) = \frac{1}{2} w^T w + w^T X \begin{pmatrix}
\lambda \\
\mu
\end{pmatrix} + \epsilon^T (K1_p - (\lambda + \alpha)) + \xi^T (K1_q - (\mu + \beta)) + b (1^T_p \lambda - 1^T_q \mu) + (\lambda^T \mu^T) 1_{p+q}.
\]

To find the dual function \(G(\lambda, \mu, \alpha, \beta)\) we minimize \(L(w, \epsilon, \xi, b, \lambda, \mu, \alpha, \beta)\) with respect to \(w, \epsilon, \xi\) and \(b\). Since the Lagrangian is convex and \((w, \epsilon, \xi, b) \in \mathbb{R}^n \times \mathbb{R}^p \times \mathbb{R}^q \times \mathbb{R}\), a convex open set, by Theorem 21.11, the Lagrangian has a minimum in \((w, \epsilon, \xi, b)\) iff \(\nabla L_{w, \epsilon, \xi, b} = 0\), so we compute its gradient with respect to \(w, \epsilon, \xi\) and \(b\) and we get

\[
\nabla L_{w, \epsilon, \xi, b} = \begin{pmatrix}
w + X \begin{pmatrix}
\lambda \\
\mu
\end{pmatrix} \\
K1_p - (\lambda + \alpha) \\
K1_q - (\mu + \beta) \\
1^T_p \lambda - 1^T_q \mu
\end{pmatrix}.
\]

By setting \(\nabla L_{w, \epsilon, \xi, b} = 0\) we get the equations

\[
w = -X \begin{pmatrix}
\lambda \\
\mu
\end{pmatrix} \quad (\star_w)
\]

and

\[
\lambda + \alpha = K1_p \\
\mu + \beta = K1_q \\
1^T_p \lambda = 1^T_q \mu.
\]

The first and the fourth equation are identical to the equations \((\star_1)\) and \((\star_2)\) that we obtained in Example 31.8. Since \(\lambda, \mu, \alpha, \beta \geq 0\), the second and the third equation are equivalent to the box constraints

\[
0 \leq \lambda_i, \mu_j \leq K, \quad i = 1, \ldots, p, \quad j = 1, \ldots, q.
\]

Using the equations that we just derived, after simplifications we get

\[
G(\lambda, \mu, \alpha, \beta) = -\frac{1}{2} (\lambda^T \mu^T) X^T X \begin{pmatrix}
\lambda \\
\mu
\end{pmatrix} + (\lambda^T \mu^T) 1_{p+q},
\]
which is independent of $\alpha$ and $\beta$ and is identical to the dual function obtained in $(*)_4$ of Example 31.8. To be perfectly rigorous,

$$G(\lambda, \mu) = \begin{cases} -\frac{1}{2} \left( \lambda^\top \mu^\top \right) X^\top X \begin{pmatrix} \lambda \\ \mu \end{pmatrix} + \begin{pmatrix} \lambda^\top \\ \mu^\top \end{pmatrix} 1_{p+q} & \text{if } \begin{cases} \sum_{i=1}^p \lambda_i = \sum_{j=1}^q \mu_j \\ 0 \leq \lambda_i \leq K, \ i = 1, \ldots, p \\ 0 \leq \mu_j \leq K, \ j = 1, \ldots, q \end{cases} \\ -\infty & \text{otherwise.} \end{cases}$$

As in Example 31.8, the dual program can be formulated as

$$\begin{align*} \text{maximize} & \quad -\frac{1}{2} \left( \lambda^\top \mu^\top \right) X^\top X \begin{pmatrix} \lambda \\ \mu \end{pmatrix} + \begin{pmatrix} \lambda^\top \\ \mu^\top \end{pmatrix} 1_{p+q} \\ \text{subject to} & \quad \sum_{i=1}^p \lambda_i = \sum_{j=1}^q \mu_j \\ & \quad 0 \leq \lambda_i \leq K, \ i = 1, \ldots, p \\ & \quad 0 \leq \mu_j \leq K, \ j = 1, \ldots, q, \end{align*}$$

or equivalently

$$\begin{align*} \text{minimize} & \quad \frac{1}{2} \left( \lambda^\top \mu^\top \right) X^\top X \begin{pmatrix} \lambda \\ \mu \end{pmatrix} - \begin{pmatrix} \lambda^\top \\ \mu^\top \end{pmatrix} 1_{p+q} \\ \text{subject to} & \quad \sum_{i=1}^p \lambda_i = \sum_{j=1}^q \mu_j \\ & \quad 0 \leq \lambda_i \leq K, \ i = 1, \ldots, p \\ & \quad 0 \leq \mu_j \leq K, \ j = 1, \ldots, q. \end{align*}$$

The dual program is solved by making use of numerical procedures based on gradient descent. If the primal problem is solvable, this yields solutions for $\lambda$ and $\mu$.

Remark: The hard margin Problem (SVM$_{h2}$) corresponds to the special case of Problem (SVM$_{s2}$) in which $\epsilon = 0$, $\xi = 0$, and $K = +\infty$. Indeed, in Problem (SVM$_{h2}$) the terms involving $\epsilon$ and $\xi$ are missing from the Lagrangian and the effect is that the box constraints are missing; we simply have $\lambda_i \geq 0$ and $\mu_j \geq 0$.

We can use the dual program to solve the primal. Once $\lambda \geq 0, \mu \geq 0$ have been found, $w$ is given by

$$w = \sum_{i=1}^p \lambda_i u_i - \sum_{j=1}^q \mu_j v_j.$$
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The complementary slackness conditions yield a classification of the points in terms of the values of λ and μ. Indeed, we have \( \epsilon_i \alpha_i = 0 \) for \( i = 1, \ldots, p \) and \( \xi_j \beta_j = 0 \) for \( j = 1, \ldots, q \). Also, if \( \lambda_i > 0 \), then corresponding constraint is active, and similarly if \( \mu_j > 0 \). Since \( \lambda_i + \alpha_i = K \), it follows that \( \epsilon_i \alpha_i = 0 \) iff \( \epsilon_i (K - \lambda_i) = 0 \), and since \( \mu_j + \beta_j = K \), we have \( \xi_j \beta_j = 0 \) iff \( \xi_j (K - \mu_j) = 0 \). Thus if \( \epsilon_i > 0 \) then \( \lambda_i = K \), and if \( \xi_j > 0 \), then \( \mu_j = K \). Consequently, if \( \lambda_i < K \) then \( \epsilon_i = 0 \) and \( u_i \) is correctly classified, and similarly if \( \mu_j < K \) then \( \xi_j = 0 \) and \( v_j \) is correctly classified. We have the following classification:

1. If \( 0 < \lambda_i < K \) then \( u_i \) is on the margin and is classified correctly. Similarly, if \( 0 < \mu_j < K \) then \( v_j \) is on the margin and is classified correctly.

2. If \( \lambda_i = K \), then if \( \epsilon_i \leq 1 \) the point \( u_i \) may be classified correctly or it lies within the margin on the correct side, but if \( \epsilon_i > 1 \) then it is misclassified. Similarly, if \( \mu_j = K \), then if \( \xi_j \leq 1 \) the point \( v_j \) may be classified correctly or it lies within the margin on the correct side, but if \( \xi_j > 1 \) then it is misclassified.

3. If \( \lambda_i = 0 \) then \( u_i \) is classified correctly. Similarly, if \( \mu_j = 0 \) then \( v_j \) is classified correctly.

If the primal has a solution \( w \neq 0 \), then the equation

\[
w = \sum_{i=1}^{p} \lambda_i u_i - \sum_{j=1}^{q} \mu_j v_j
\]

implies that either there is some index \( i_0 \) such that \( \lambda_{i_0} > 0 \) or there is some index \( j_0 \) such that \( \mu_{j_0} > 0 \). The constraint

\[
\sum_{i=1}^{p} \lambda_i = \sum_{j=1}^{q} \mu_j
\]

implies that there is some index \( i_0 \) such that \( \lambda_{i_0} > 0 \) and there is some index \( j_0 \) such that \( \mu_{j_0} > 0 \). However, a priori, nothing prevents the situation where \( \lambda_i = K \) for all nonzero \( \lambda_i \) or \( \mu_j = K \) for all nonzero \( \mu_j \). If this happens, we can rerun the optimization method with a larger value of \( K \). Observe that the equation

\[
\sum_{i=1}^{p} \lambda_i = \sum_{j=1}^{q} \mu_j
\]

implies that if there is some index \( i_0 \) such that \( 0 < \lambda_{i_0} < K \), then there is some index \( j_0 \) such that \( 0 < \mu_{j_0} < K \), and vice-versa. If the following mild hypothesis holds, then \( b \) can be found.

**Standard Margin Hypothesis** for (SVMs). There is some index \( i_0 \) such that \( 0 < \lambda_{i_0} < K \) and there is some index \( j_0 \) such that \( 0 < \mu_{j_0} < K \). This means that some \( u_{i_0} \) is correctly classified and on the blue margin, and some \( v_{j_0} \) is correctly classified and on the red margin.
If the **Standard Margin Hypothesis** for \((\text{SVM}_{s2})\) holds then \(\epsilon_{i_0} = 0\) and \(\mu_{j_0} = 0\), and then we have the active equations
\[
w^\top u_i - b = 1 \quad \text{and} \quad -w^\top v_j + b = 1,
\]
and we obtain
\[
b = \frac{1}{2}(w^\top u_{i_0} + w^\top v_{j_0}).
\]

**Remark:** There is a cheap version of Problem \((\text{SVM}_{s2})\) which consists in dropping the term \((1/2)w^\top w\) from the objective function:

**Soft margin classifier** \((\text{SVM}_{s2})\):

\[
\text{minimize} \quad \sum_{i=1}^p \epsilon_i + \sum_{j=1}^q \xi_j
\]
subject to
\[
w^\top u_i - b \geq 1 - \epsilon_i, \quad \epsilon_i \geq 0 \quad i = 1, \ldots, p
\]
\[-w^\top v_j + b \geq 1 - \xi_j, \quad \xi_j \geq 0 \quad j = 1, \ldots, q.
\]

The above program is a linear program that minimizes the number of misclassified points but does not care about enforcing a minimum margin. An example of its use is given in Boyd and Vandenberghe; see [22], Section 8.6.1.

The “kernelized” version of Problem \((\text{SVM}_{s2})\) is the following:

**Soft margin kernel SVM** \((\text{SVM}_{s2})\):

\[
\text{minimize} \quad \frac{1}{2} \langle w, w \rangle + K\left(\epsilon^\top \quad \xi^\top\right) 1_{p+q}
\]
subject to
\[
\langle w, \varphi(u_i) \rangle - b \geq 1 - \epsilon_i, \quad \epsilon_i \geq 0 \quad i = 1, \ldots, p
\]
\[-\langle w, \varphi(v_j) \rangle + b \geq 1 - \xi_j, \quad \xi_j \geq 0 \quad j = 1, \ldots, q.
\]

Redoing the computation of the dual function, we find that the dual program is given by

\[
\text{minimize} \quad \frac{1}{2} \left(\lambda^\top \quad \mu^\top\right) K \left(\lambda \mu\right) - \left(\lambda^\top \quad \mu^\top\right) 1_{p+q}
\]
subject to
\[
\sum_{i=1}^p \lambda_i = \sum_{j=1}^q \mu_j
\]
\[0 \leq \lambda_i \leq K, \quad i = 1, \ldots, p \]
\[0 \leq \mu_j \leq K, \quad j = 1, \ldots, q.
\]
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where \(K\) is the \(\ell \times \ell\) kernel symmetric matrix (with \(\ell = p + q\)) given at the end of Section 34.1. We also find that

\[
w = \sum_{i=1}^{p} \lambda_i \varphi(u_i) - \sum_{j=1}^{q} \mu_j \varphi(v_j),
\]

so

\[
b = \frac{1}{2} \left( \sum_{i=1}^{p} \lambda_i (\kappa(u_i, u_{i0}) + \kappa(u_i, v_{j0})) - \sum_{j=1}^{q} \mu_j (\kappa(v_j, u_{i0}) + \kappa(v_j, v_{j0})) \right),
\]

and the classification function

\[
f(x) = \text{sgn}(\langle w, \varphi(x) \rangle - b)
\]

is given by

\[
f(x) = \text{sgn} \left( \sum_{i=1}^{p} \lambda_i (2\kappa(u_i, x) - \kappa(u_i, u_{i0}) - \kappa(u_i, v_{j0}))
- \sum_{j=1}^{q} \mu_j (2\kappa(v_j, x) - \kappa(v_j, u_{i0}) - \kappa(v_j, v_{j0})) \right).
\]

17.3 Soft Margin Support Vector Machines; \((\text{SVM}_{s2'})\)

In this section we consider a generalization of Problem \((\text{SVM}_{s2'})\) for a version of the soft margin SVM coming from Problem \((\text{SVM}_{h2})\), by adding an extra degree of freedom, namely instead of the margin \(\delta = 1/\|w\|\), we use the margin \(\delta = \eta/\|w\|\) where \(\eta\) is some positive constant that we wish to maximize. To do so, we add a term \(-K_m \eta\) to the objective function \((1/2)w^\top w\) as well as the “regularizing term” \(K_s \left( \sum_{i=1}^{p} \epsilon_i + \sum_{j=1}^{q} \xi_j \right)\) whose purpose is to make \(\epsilon\) and \(\xi\) sparse, where \(K_m > 0\) and \(K_s > 0\) are fixed constants that can be adjusted to determine the influence of \(\eta\) and the regularizing term.

**Soft margin SVM \((\text{SVM}_{s2'})\):**

\[
\text{minimize} \quad \frac{1}{2} w^\top w - K_m \eta + K_s \left( \epsilon^\top + \xi^\top \right) 1_{p+q}
\]

subject to

\[
w^\top u_i - b \geq \eta - \epsilon_i, \quad \epsilon_i \geq 0 \quad i = 1, \ldots, p
\]

\[
-w^\top v_j + b \geq \eta - \xi_j, \quad \xi_j \geq 0 \quad j = 1, \ldots, q
\]

\[
\eta \geq 0.
\]

This version of the SVM problem was first discussed in Schölkopf, Smola, Williamson, and Bartlett [88] under the name of \(\nu\)-SVC (or \(\nu\)-SVM), and also used in Schölkopf, Platt,
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Shawe–Taylor, and Smola [87]. The \( \nu \)-SVC method is also presented in Schölkopf and Smola [86] (which contains much more). The difference between the \( \nu \)-SVC method and the method presented in Section 34.2, sometimes called the \( C \)-SVM method, was thoroughly investigated by Chan and Lin [27].

For this problem, it is no longer clear that if \((w, \eta, b, \epsilon, \xi)\) is an optimal solution, then \(w \neq 0\) and \(\eta > 0\). In fact, if the sets of points are not linearly separable and if \(K_s\) is chosen too big, Problem (SVM\(_{s2'}\)) may fail to have an optimal solution.

We show that in order for the problem to have a solution we must pick \(K_m\) and \(K_s\) so that

\[
K_m \leq \min\{2pK_s, 2qK_s\}.
\]

If we define \(\nu\) by

\[
\nu = \frac{K_m}{(p+q)K_s},
\]

then \(K_m \leq \min\{2pK_s, 2qK_s\}\) is equivalent to

\[
\nu \leq \min\left\{ \frac{2p}{p+q}, \frac{2q}{p+q} \right\} \leq 1.
\]

The reason for introducing \(\nu\) is that \(\nu(p+q)/2\) can be interpreted as a the maximum number of points failing to achieve the margin \(\eta\). If the sets \(\{u_i\}\) and \(\{v_j\}\) are not linearly separable, then we must pick \(\nu\) so that \(\nu \geq 2/(p+q)\) for the method to have an optimal solution. If \(\nu < 3/(p+q)\) and at least three points are misclassified then we have some interesting guarantees; see Proposition 34.5 and Proposition 34.6.

The objective function of our problem is convex and the constraints are affine. Consequently, by Theorem 31.14(2) if the primal problem (SVM\(_{s2'}\)) has an optimal solution, then the dual problem has a solution too, and the duality gap is zero. This does not immediately imply that an optimal solution of the dual yields an optimal solution of the primal because the hypotheses of Theorem 31.14(1) fail to hold.

We show that if the primal problem has an optimal solution \((w, \eta, \epsilon, \xi, b)\) with \(w \neq 0\), then any optimal solution of the dual problem determines \(\lambda\) and \(\mu\), which in turn determine \(w\) via the equation

\[
w = -X (\lambda \mu) = \sum_{i=1}^{p} \lambda_i u_i - \sum_{j=1}^{q} \mu_j v_j, \quad \text{(**}_w\text{)}
\]

and \(\eta \geq 0\).

It remains to determine \(b, \eta, \epsilon\) and \(\xi\). The solution of the dual does not determine \(b, \eta, \epsilon, \xi\) directly, and we are not aware of necessary and sufficient conditions that ensure that they can be determined. The best we can do is to use the KKT conditions.

The simplest sufficient condition is what we call the
17.3. **SOFT MARGIN SUPPORT VECTOR MACHINES; (SVM\(_{s^2}\))**

**Standard Margin Hypothesis** for (SVM\(_{s^2}\)): There is some \(i_0\) such that \(0 < \lambda_{i_0} < K_s\) and there is some \(j_0\) such that \(0 < \mu_{j_0} < K_s\). This means that some \(u_{i_0}\) is correctly classified and on the blue margin, and some \(v_{j_0}\) is correctly classified and on the red margin.

In this case, then by complementary slackness it can be shown that \(\epsilon_{i_0} = 0\), \(\xi_{i_0} = 0\), and the corresponding inequalities are active, that is we have the equations

\[
\begin{align*}
w^\top u_{i_0} - b &= \eta, \\
-w^\top v_{j_0} + b &= \eta,
\end{align*}
\]

so we can solve for \(b\) and \(\eta\). Then, since by complementary slackness if \(\epsilon_i > 0\) then \(\lambda_i = K_s\) and if \(\xi_j > 0\) then \(\mu_j = K_s\), all inequalities corresponding to such \(\epsilon_i > 0\) and \(\mu_j > 0\) are active, and we can solve for \(\epsilon_i\) and \(\xi_j\).

If \(2/(p + q) \leq \nu < 3/(p + q)\) and at least three points are misclassified then we can guarantee that either there is some \(i_0\) such that the constraint \(w^\top u_{i_0} - b = \eta\) is active or there is some \(j_0\) such that the constraint \(-w^\top v_{j_0} + b = \eta\) is active.

If \((w, \eta, \epsilon, \xi, b)\) is an optimal solution of Problem (SVM\(_{s^2}\)) with \(w \neq 0\), then the points \(u_i\) and \(v_j\) are classified as follows:

(1) If \(\epsilon_i = 0\), then the point \(u_i\) is correctly classified and is either on the blue margin (the hyperplane \(H_{w,b+\eta}\) of equation \(w^\top x = b + \eta\)) or on the correct side of the blue margin (the blue side). Similarly, if \(\xi_j = 0\), then the point \(v_j\) is correctly classified and is either on the red margin (the hyperplane \(H_{w,b-\eta}\) of equation \(w^\top x = b - \eta\)) or on the correct side of the red margin (the red side).

(2) If \(0 < \epsilon_i \leq \eta\), then the point \(u_i\) lies inside the margin (the slab), but on the correct side of the separating hyperplane (the blue side). If \(\epsilon_i = \eta\), then \(u_i\) lies on the separating hyperplane. Similarly, if \(0 < \xi_j \leq \eta\), then the point \(v_j\) lies inside the margin (the slab), but on the correct side of the separating hyperplane (the red side). If \(\xi_j = \eta\), then \(v_j\) lies on the separating hyperplane.

(3) If \(\epsilon_i > \eta\), then the point \(u_i\) lies on the wrong side of the separating hyperplane (the red side); it is misclassified. Similarly, if \(\xi_j > \eta\), then the point \(v_j\) lies on the wrong side of the separating hyperplane (the blue side); it is misclassified.

Points for which \(\epsilon_i > 0\) (or \(\xi_j > 0\)) are called *margin-errors*; they either lie within the slab or they are misclassified.

The linear constraints are given by the \((2(p + q) + 1) \times (n + p + q + 2)\) matrix given in block form by

\[
C = \begin{pmatrix}
X^\top & -I_{p+q} & 1_p & 1_{p+q} \\
0_{p+q,n} & -I_{p+q} & 0_{p+q} & 0_{p+q} \\
0_n^\top & 0_{p+q}^\top & 0 & -1
\end{pmatrix},
\]
and the linear constraints are expressed by
\[
\begin{pmatrix}
X \top & -I_{p+q} & 1_p \\
-1_q & I_{p+q} \\
0_{p+q,n} & 0_{p+q} & 0
\end{pmatrix}
\begin{pmatrix}
w \\
\epsilon \\
\xi \\
0 \\
b
\eta
\end{pmatrix}
\leq
\begin{pmatrix}
0_{p+q} \\
0
\end{pmatrix}.
\]

The objective function is given by
\[
J(w, \epsilon, \xi, b, \eta) = \frac{1}{2} w \top w - K_m \eta + K_s (\epsilon \top \xi \top) 1_{p+q}.
\]

The Lagrangian \(L(w, \epsilon, \xi, b, \eta, \lambda, \mu, \alpha, \beta, \gamma)\) with \(\lambda, \alpha \in \mathbb{R}_+^{p}, \mu, \beta \in \mathbb{R}_+^{q},\) and \(\gamma \in \mathbb{R}_+\) is given by
\[
L(w, \epsilon, \xi, b, \eta, \lambda, \mu, \alpha, \beta, \gamma) = \frac{1}{2} w \top w - K_m \eta + K_s (\epsilon \top \xi \top) 1_{p+q} + (w \top (\epsilon \top \xi \top) b \eta) C \top \begin{pmatrix}
\lambda \\
\mu \\
\alpha \\
\beta \\
\gamma
\end{pmatrix}.
\]

Since
\[
(w \top (\epsilon \top \xi \top) b \eta) C \top \begin{pmatrix}
\lambda \\
\mu \\
\alpha \\
\beta \\
\gamma
\end{pmatrix} = w \top X \begin{pmatrix}
\lambda \\
\mu \\
\alpha \\
\beta \\
\gamma
\end{pmatrix} - \epsilon \top (\lambda + \alpha) - \xi \top (\mu + \beta) + b(1_p \top \lambda - 1_q \top \mu)
\]
\[
+ \eta (1_p \top \lambda + 1_q \top \mu) - \gamma \eta,
\]
the Lagrangian can be written as
\[
L(w, \epsilon, \xi, b, \eta, \lambda, \mu, \alpha, \beta, \gamma) = \frac{1}{2} w \top w - K_m \eta + K_s (\epsilon \top \xi \top) 1_{p+q} + w \top X \begin{pmatrix}
\lambda \\
\mu \\
\alpha \\
\beta \\
\gamma
\end{pmatrix} - \epsilon \top (\lambda + \alpha) - \xi \top (\mu + \beta) + b(1_p \top \lambda - 1_q \top \mu)
\]
\[
+ \eta (1_p \top \lambda + 1_q \top \mu - K_m - \gamma) \eta
\]
\[
+ \epsilon \top (K_s 1_p - (\lambda + \alpha)) + \xi \top (K_s 1_q - (\mu + \beta)) + b(1_p \top \lambda - 1_q \top \mu).
\]

To find the dual function \(G(\lambda, \mu, \alpha, \beta, \gamma)\) we minimize \(L(w, \epsilon, \xi, b, \eta, \lambda, \mu, \alpha, \beta, \gamma)\) with respect to \(w, \epsilon, \xi, b,\) and \(\eta.\) Since the Lagrangian is convex and \((w, \epsilon, \xi, b, \eta) \in \mathbb{R}^n \times \mathbb{R}^p \times \mathbb{R}^q \times \)
\[ R \times R, \text{ a convex open set, by Theorem 21.11, the Lagrangian has a minimum in } (w, \epsilon, \xi, b, \eta) \text{ iff } \nabla L_{w,\epsilon,\xi,b,\eta} = 0, \] so we compute its gradient with respect to \( w, \epsilon, \xi, b, \eta \) and we get

\[
\nabla L_{w,\epsilon,\xi,b,\eta} = \begin{pmatrix}
X \begin{pmatrix} \lambda \\ \mu \end{pmatrix} + w \\
K_s 1_p - (\lambda + \alpha) \\
K_s 1_q - (\mu + \beta) \\
1_p^\top \lambda - 1_q^\top \mu \\
1_p^\top \lambda + 1_q^\top \mu - K_m - \gamma
\end{pmatrix}.
\]

By setting \( \nabla L_{w,\epsilon,\xi,b,\eta} = 0 \) we get the equations

\[
w = -X \begin{pmatrix} \lambda \\ \mu \end{pmatrix} \quad (\ast_w)
\]

\[
\lambda + \alpha = K_s 1_p \\
\mu + \beta = K_s 1_q \\
1_p^\top \lambda = 1_q^\top \mu,
\]

and

\[
1_p^\top \lambda + 1_q^\top \mu = K_m + \gamma. \quad (\ast_\gamma)
\]

The second and third equations are equivalent to the box constraints

\[
0 \leq \lambda_i, \mu_j \leq K_s, \quad i = 1, \ldots, p, \ j = 1, \ldots, q,
\]

and since \( \gamma \geq 0 \) equation (\ast_\gamma) is equivalent to

\[
1_p^\top \lambda + 1_q^\top \mu \geq K_m.
\]

Plugging back \( w \) from (\ast_w) into the Lagrangian, after simplifications we get

\[
G(\lambda, \mu, \alpha, \beta) = \frac{1}{2} \begin{pmatrix} \lambda^\top & \mu^\top \end{pmatrix} X^\top X \begin{pmatrix} \lambda \\ \mu \end{pmatrix} - (\lambda^\top \mu^\top) \begin{pmatrix} \lambda \\ \mu \end{pmatrix}
= -\frac{1}{2} \begin{pmatrix} \lambda^\top & \mu^\top \end{pmatrix} X^\top X \begin{pmatrix} \lambda \\ \mu \end{pmatrix},
\]

so the dual function is independent of \( \alpha, \beta \) and is given by

\[
G(\lambda, \mu) = -\frac{1}{2} \begin{pmatrix} \lambda^\top & \mu^\top \end{pmatrix} X^\top X \begin{pmatrix} \lambda \\ \mu \end{pmatrix}.
\]
The dual program is given by

\[
\text{maximize} \quad -\frac{1}{2} \begin{pmatrix} \lambda^T & \mu^T \end{pmatrix} X^T X \begin{pmatrix} \lambda \\ \mu \end{pmatrix}
\]

subject to

\[
\begin{align*}
\sum_{i=1}^{p} \lambda_i &= \sum_{j=1}^{q} \mu_j \\
\sum_{i=1}^{p} \lambda_i + \sum_{j=1}^{q} \mu_j &\geq K_m \\
0 \leq \lambda_i &\leq K_s, \quad i = 1, \ldots, p \\
0 \leq \mu_j &\leq K_s, \quad j = 1, \ldots, q.
\end{align*}
\]

Finally, the dual program is equivalent to the following minimization program:

\[
\text{minimize} \quad \frac{1}{2} \begin{pmatrix} \lambda^T & \mu^T \end{pmatrix} X^T X \begin{pmatrix} \lambda \\ \mu \end{pmatrix}
\]

subject to

\[
\begin{align*}
\sum_{i=1}^{p} \lambda_i &= \sum_{j=1}^{q} \mu_j \\
\sum_{i=1}^{p} \lambda_i + \sum_{j=1}^{q} \mu_j &\geq K_m \\
0 \leq \lambda_i &\leq K_s, \quad i = 1, \ldots, p \\
0 \leq \mu_j &\leq K_s, \quad j = 1, \ldots, q.
\end{align*}
\]

The dual program is solved by making use of numerical procedures based on gradient descent. If the primal problem is solvable, this yields solutions for \( \lambda \) and \( \mu \). Once a solution for \( \lambda \) and \( \mu \) is obtained, we have

\[
w = - X \begin{pmatrix} \lambda \\ \mu \end{pmatrix} = \sum_{i=1}^{p} \lambda_i u_i - \sum_{j=1}^{q} \mu_j v_j.
\]

As we said earlier, the hypotheses of Theorem 31.14(2) hold, so if the primal problem (\( \text{SVM}_{s2'} \)) has an optimal solution with \( w \neq 0 \), then the dual problem has a solution too, and the duality gap is zero. Therefore, for optimal solutions we have

\[
L(w, \epsilon, \xi, b, \eta, \lambda, \mu, \alpha, \beta, \gamma) = G(\lambda, \mu, \alpha, \beta, \gamma),
\]

which means that

\[
\frac{1}{2} w^T w - K_m \eta + K_s \left( \sum_{i=1}^{p} \epsilon_i + \sum_{j=1}^{q} \xi_j \right) = -\frac{1}{2} \begin{pmatrix} \lambda^T & \mu^T \end{pmatrix} X^T X \begin{pmatrix} \lambda \\ \mu \end{pmatrix},
\]
and since
\[ w = -X \begin{pmatrix} \lambda \\ \mu \end{pmatrix} \]
we get
\[ \frac{1}{2} \begin{pmatrix} \lambda^T & \mu^T \end{pmatrix} X^T X \begin{pmatrix} \lambda \\ \mu \end{pmatrix} - K_m \eta + K_s \left( \sum_{i=1}^{p} \epsilon_i + \sum_{j=1}^{q} \xi_j \right) = \frac{1}{2} \begin{pmatrix} \lambda^T & \mu^T \end{pmatrix} X^T X \begin{pmatrix} \lambda \\ \mu \end{pmatrix}, \]
which yields
\[ \eta = \frac{K_s}{K_m} \left( \sum_{i=1}^{p} \epsilon_i + \sum_{j=1}^{q} \xi_j \right) + \frac{1}{K_m} \begin{pmatrix} \lambda^T & \mu^T \end{pmatrix} X^T X \begin{pmatrix} \lambda \\ \mu \end{pmatrix}. \] (*)
Therefore, \( \eta \geq 0. \)

**Remarks:**

(1) The objective function of Problem (SVM_{s2'}) is half of the objective function of Problem (SVM_{s1}), but some of the constraints are different. However, the major advantage of Problem (SVM_{s2'}) is that \( w \) is always determined.

(2) Since we proved that if the primal problem (SVM_{s2'}) has an optimal solution with \( w \neq 0 \) then \( \eta \geq 0 \), one might wonder why the constraint \( \eta \geq 0 \) was included. If we delete this constraint, it is easy to see that the only difference is that instead of the equation
\[ 1_p^T \lambda + 1_q^T \mu = K_m + \gamma \]
we obtain the equation
\[ 1_p^T \lambda + 1_q^T \mu = K_m. \]
Since the equation
\[ 1_p^T \lambda = 1_q^T \mu \]
holds, in the first case we obtain
\[ 1_p^T \lambda = 1_q^T \mu = \frac{K_m}{2} + \frac{\gamma}{2}, \] (\( \ast_1 \))
and in the second case, we obtain
\[ 1_p^T \lambda = 1_q^T \mu = \frac{K_m}{2}. \] (\( \ast_2 \))
If \( \eta > 0 \), then by complementary slackness \( \gamma = 0 \), in which case (\( \ast_1 \)) and (\( \ast_2 \)) are equivalent. But if \( \eta = 0 \), then \( \gamma \) could be strictly positive.
It not clear that the option to include the constraint $\eta \geq 0$ in the primal is advantageous, except perhaps for the fact that in the dual program the equation and inequality

$$1_p^\top \lambda + 1_q^\top \mu \geq K_m$$

are included rather than the equations

$$1_p^\top \lambda = 1_q^\top \mu = \frac{K_m}{2}.$$ 

Perhaps the use of an inequality makes it easier to solve the dual. To settle this issue it seems that we need to run practical solvers on some test data.

Returning to Problem (SVM$_{s'}$), the complementary slackness conditions yield a classification of the points in terms of the values of $\lambda$ and $\mu$. Indeed, we have $\epsilon_i\alpha_i = 0$ for $i = 1, \ldots, p$ and $\xi_j\beta_j = 0$ for $j = 1, \ldots, q$. Also, if $\lambda_i > 0$, then the corresponding constraint is active, and similarly if $\mu_j > 0$. Since $\lambda_i + \alpha_i = K_s$, it follows that $\epsilon_i\alpha_i = 0$ iff $\epsilon_i(K_s - \lambda_i) = 0$, and since $\mu_j + \beta_j = K_s$, we have $\xi_j\beta_j = 0$ iff $\xi_j(K_s - \mu_j) = 0$. Thus if $\epsilon_i > 0$ then $\lambda_i = K_s$, and if $\xi_j > 0$, then $\mu_j = K_s$. Consequently, if $\lambda_i < K_s$ then $\epsilon_i = 0$ and $u_i$ is correctly classified, and similarly if $\mu_j < K_s$ then $\xi_j = 0$ and $v_j$ is correctly classified.

In addition to the constraints

$$0 \leq \lambda_i \leq K_s, \quad 0 \leq \mu_j \leq K_s,$$

we also have the constraints

$$\sum_{i=1}^{p} \lambda_i = \sum_{j=1}^{q} \mu_j$$

and

$$\sum_{i=1}^{p} \lambda_i + \sum_{j=1}^{q} \mu_j \geq K_m$$

which imply that

$$\sum_{i=1}^{p} \lambda_i \geq \frac{K_m}{2} \quad \text{and} \quad \sum_{j=1}^{q} \mu_j \geq \frac{K_m}{2}. \quad (***)$$

Since $\lambda, \mu$ are all nonnegative, if $\lambda_i = K_s$ for all $i$ and if $\mu_j = K_s$ for all $j$ then

$$\frac{K_m}{2} \leq \sum_{i=1}^{p} \lambda_i \leq pK_s$$

and

$$\frac{K_m}{2} \leq \sum_{j=1}^{q} \mu_j \leq qK_s,$$
so these constraints are not satisfied unless \( K_m \leq \min\{2pK_s, 2qK_s\} \), so we assume that \( K_m \leq \min\{2pK_s, 2qK_s\} \). The equations in (†) also imply that there is some \( i_0 \) such that \( \lambda_{i_0} > 0 \) and some \( j_0 \) such that \( \mu_{j_0} > 0 \).

We have the following classification (recall that \( \eta > 0 \)):

1. If \( 0 < \lambda_i < K_s \) then \( u_i \) is on the margin and is classified correctly. Similarly, if \( 0 < \mu_j < K_s \) then \( v_j \) is on the margin and is classified correctly.

2. If \( \lambda_i = K_s \), then we can’t say more without looking at \( \epsilon_i \). If \( \epsilon_i = 0 \) then the point \( u_i \) is on the margin and is classified correctly, and if \( 0 < \epsilon_i \leq \eta \), then \( u_i \) lies within the margin on the correct side, but if \( \epsilon_i > \eta \) then it is misclassified. Similarly, if \( \mu_j = K_s \), then we can’t say more without looking at \( \xi_j \). If \( \xi_j = 0 \) then the point \( v_j \) is on the margin and is classified correctly, and if \( 0 < \xi_j \leq \eta \), then \( v_j \) lies within the margin on the correct side, but if \( \xi_j > \eta \) then it is misclassified.

3. If \( \lambda_i = 0 \) then \( u_i \) is classified correctly. Similarly, if \( \mu_j = 0 \) then \( v_j \) is classified correctly. There is no way to tell whether \( u_i \) is on the margin or not, and similarly for \( v_j \).

We find it convenient to define \( \nu > 0 \) such that

\[
K_m = (p + q)K_s \nu,
\]

that is

\[
\nu = \frac{K_m}{(p + q)K_s},
\]

so that the objective function \( J(w, \epsilon, \xi, b, \eta) \) is given by

\[
J(w, \epsilon, \xi, b, \eta) = \frac{1}{2} w^\top w + K \left( -\nu \eta + \frac{1}{p + q} (\epsilon^\top \xi^\top) 1_{p+q} \right),
\]

with \( K = (p + q)K_s \), and so \( K_m = K \nu \) and \( K_s = K/(p + q) \).

Observe that the condition \( K_m \leq \min\{2pK_s, 2qK_s\} \) is equivalent to

\[
\nu \leq \min\left\{ \frac{2p}{p + q}, \frac{2q}{p + q} \right\} \leq 1,
\]

and the condition \( K_s \leq K_m/2 \) is equivalent to

\[
\frac{2}{p + q} \leq \nu.
\]

Since we obtain an equivalent problem by rescaling by a common positive factor, it is convenient to normalize \( K_s \) as

\[
K_s = \frac{1}{p + q},
\]
in which case \( K_m = \nu \). This method is called the \( \nu \)-support vector machine.

Under the Standard Margin Hypothesis for \( (\text{SVM}_{s^2}) \), there is some \( i_0 \) such that \( 0 < \lambda_{i_0} < K_s \) and some \( j_0 \) such that \( 0 < \mu_{j_0} < K_s \), and by the complementary slackness conditions \( \epsilon_{i_0} = 0 \) and \( \xi_{j_0} = 0 \), so we have the two active constraints

\[
w^\top u_{i_0} - b = \eta, \quad -w^\top v_{j_0} + b = \eta,
\]

and we can solve for \( b \) and \( \eta \) and we get

\[
b = \frac{w^\top u_{i_0} + w^\top v_{j_0}}{2},
\]

\[
\eta = \frac{w^\top u_{i_0} - w^\top v_{j_0}}{2}.
\]

The equations (†) and the box inequalities

\[
0 \leq \lambda_i \leq K_s, \quad 0 \leq \mu_j \leq K_s
\]

also imply the following facts:

**Proposition 17.1.** If Problem \( (\text{SVM}_{s^2}) \) has an optimal solution with \( w \neq 0 \) and \( \eta > 0 \), then the following facts hold:

1. At most \( \nu(p+q)/2 \) points \( u_i \) fail to achieve the margin \( \eta \), and at most \( \nu(p+q)/2 \) points \( v_j \) fail to achieve the margin \( \eta \).

2. At least \( \nu(p+q)/2 \) points \( u_i \) have margin at most \( \eta \), and at least \( \nu(q+q)/2 \) points have margin at most \( \eta \).

**Proof.** (1) Recall that for an optimal solution with \( w \neq 0 \) and \( \eta > 0 \), we have \( \gamma = 0 \), so by (∗γ) we have the equations

\[
\sum_{i=1}^{p} \lambda_i = \frac{K_m}{2} \quad \text{and} \quad \sum_{j=1}^{q} \mu_j = \frac{K_m}{2}.
\]

If \( u_i \) fails to achieve the margin \( \eta \), then \( \epsilon_i > 0 \), and by complementary slackness \( \lambda_i = K_s = K_m/(\nu(p+q)) \), so if there are \( p_f \) such points then

\[
\frac{K_m}{2} = \sum_{i=1}^{p} \lambda_i \geq \frac{K_m p_f}{\nu(p+q)},
\]

so

\[
p_f \leq \frac{\nu(p+q)}{2}.
\]

A similar reasoning applies if \( v_j \) fails to achieve the margin \( \eta \) with \( \sum_{i=1}^{p} \lambda_i \) replaced by \( \sum_{j=1}^{q} \mu_j \) (and where \( q_f \) is the number of points \( v_j \) that fail to achieve the margin \( \eta \)).
(2) A point \( u_i \) has margin at most \( \eta \) iff \( \lambda_i > 0 \). If

\[
I_m = \{ i \in \{1, \ldots, p\} \mid \lambda_i > 0 \} \quad \text{and} \quad p_m = |I_m|,
\]

then

\[
\frac{K_m}{2} = \sum_{i=1}^{p} \lambda_i = \sum_{i \in I_m} \lambda_i,
\]

and since \( \lambda_i \leq K_s = K_m/(\nu(p + q)) \), we have

\[
\frac{K_m}{2} = \sum_{i \in I_m} \lambda_i \leq \frac{K_m p_m}{\nu(p + q)},
\]

which yields

\[
p_m \geq \frac{\nu(p + q)}{2}.
\]

A similar reasoning applies if a point \( v_j \) has margin at most \( \eta \).

Note that if \( \nu \) is chosen so that \( \nu < 2/(p + q) \), then \( \nu(p + q)/2 < 1 \), which means that none of the data points are misclassified; in other words, the \( u_i \)s and \( v_j \)s are linearly separable. Thus again, we see that if the \( u_i \)s and \( v_j \)s are not linearly separable we must pick \( \nu \) such that \( 2/(p + q) \leq \nu \leq \min\{2p/(p + q), 2q/(p + q)\} \) for the method to succeed.

The following proposition clarifies the role of the constant \( \nu \) in establishing the trade-off between the width of the margin and the number of margin-error points. In particular, it shows that if Problem (SVM\(_{\text{ SVM}}\)) has an optimal solution with \( w \neq 0 \) and if \( \nu < \min\{2p/(p + q), 2q/(p + q)\} \), then at least some \( u_i \) or some \( v_j \) is classified correctly. Obviously we have \( 2/(p + q) \leq \min\{2p/(p + q), 2q/(p + q)\} \).

**Proposition 17.2.** Suppose \((w, b, \eta, \epsilon, \xi)\) is an optimal solution of Problem (SVM\(_{\text{ SVM}}\)) with \( w \neq 0 \) and \( \eta > 0 \), and let \( p_f \) be the number of points \( u_i \) that are misclassified \((\epsilon_i > 0)\) and \( q_f \) be the number of points \( v_j \) that are misclassified \((\xi_j > 0)\). If \( p_f + q_f \geq 3 \) and if \( 2/(p + q) \leq \nu < (p_f + q_f)/(p + q) \), then either there is some \( i \) such that \( \epsilon_i = 0 \) and the constraint \( w^\top u_i - b = \eta \) is active, or there is some \( j \) such that \( \xi_j = 0 \) and the constraint \( -w^\top v_j + b = \eta \) is active.

**Proof.** (1) We may assume that \( K_s = 1/(p + q) \). We proceed by contradiction. Thus we assume that for all \( i \in \{1, \ldots, p\} \), if \( \epsilon_i = 0 \) then the constraint \( w^\top u_i - b \geq \eta \) is not active, namely \( w^\top u_i - b > \eta \), and for all \( j \in \{1, \ldots, q\} \), if \( \xi_j = 0 \) then the constraint \( -w^\top v_j + b \geq \eta \) is not active, namely \( -w^\top v_j + b > \eta \).

Let \( I = \{ i \in \{1, \ldots, p\} \mid \epsilon_i > 0 \} \), let \( J = \{ j \in \{1, \ldots, q\} \mid \xi_j > 0 \} \), and let \( p_f = |I| \) and \( q_f = |J| \) (of course, \( \eta > 0 \)).
CHAPTER 17. SOFT MARGIN SUPPORT VECTOR MACHINES

Assume that \( p_f + q_f \geq 3 \). By complementary slackness all the constraints for which \( i \in I \) and \( j \in J \) are active, so our hypotheses are

\[
\begin{align*}
    w^\top u_i - b &= \eta - \epsilon_i \quad \epsilon_i > 0 \quad i \in I \\
    -w^\top v_j + b &= \eta - \xi_j \quad \xi_j > 0 \quad j \in J \\
    w^\top u_i - b &= \eta \quad i \notin I \\
    -w^\top v_j + b &= \eta \quad j \notin J.
\end{align*}
\]

For any \( \theta > 0 \) such that

\[
\theta < \min\{\epsilon_i, \xi_j, \eta \mid i \in \{1, \ldots, p\}, j \in \{1, \ldots, q\}\},
\]
we can write

\[
\begin{align*}
    w^\top u_i - b &= \eta - \theta - (\epsilon_i - \theta) \quad \epsilon_i - \theta \geq 0 \quad i \in I \\
    -w^\top v_j + b &= \eta - \theta - (\xi_j - \theta) \quad \xi_j - \theta \geq 0 \quad j \in J \\
    w^\top u_i - b &= \eta - \theta \quad i \notin I \\
    -w^\top v_j + b &= \eta - \theta \quad j \notin J.
\end{align*}
\]

The original value of the objective function is

\[
\omega(0) = \frac{1}{2} w^\top w - \nu \eta + \frac{1}{p + q} \left( \sum_{i \in I} \epsilon_i + \sum_{j \in J} \xi_j \right),
\]

and the new value is

\[
\omega(\theta) = \frac{1}{2} w^\top w - \nu(\eta - \theta) + \frac{1}{p + q} \left( \sum_{i \in I} (\epsilon_i - \theta) + \sum_{j \in J} (\xi_j - \theta) \right)
\]

\[
= \frac{1}{2} w^\top w - \nu \eta + \frac{1}{p + q} \left( \sum_{i \in I} \epsilon_i + \sum_{j \in J} \xi_j \right) - \left( \frac{p_f + q_f}{p + q} - \nu \right) \theta.
\]

Since by hypothesis \( p_f + q_f \geq 3 \), if

\[
\frac{2}{p + q} \leq \nu < \frac{p_f + q_f}{p + q},
\]

then the term involving \( \theta \) is negative so

\[
\omega(\theta) < \omega(0),
\]

and by the choice of \( \theta \) we have \( \eta - \theta > 0 \), so \((w, b, \eta - \theta, \epsilon - \theta, \xi - \theta)\) is a feasible solution, contradicting the optimality of the solution \((w, b, \eta, \epsilon, \xi)\); here we write \( \epsilon - \theta \) for the vector \((\epsilon_1 - \theta, \ldots, \epsilon_p - \theta)\), and similarly for \( \xi - \theta \).

\[\square\]
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Note that if \( p_f + q_f = p + q \) and \( \nu < \min\{2p/(p+q), 2q/(p+q)\} \leq 1 \), then Proposition 34.5 yields a contradiction. Therefore \( p_f + q_f < p + q \), that is, at least some \( u_i \) or some \( v_j \) is classified correctly.

**Remark:** If the the sets \( \{u_i\} \) and \( \{v_j\} \) are linearly separable, then we know from Theorem 31.10 that some \( u_i \) is on the blue margin and some \( v_j \) is on the red margin.

We also have the following proposition that gives a sufficient condition implying that \( \eta \) and \( b \) can be determined from an optimal solution \( (\lambda, \mu) \) of the dual.

**Proposition 17.3.** If \((w, b, \eta, \epsilon, \xi)\) is an optimal solution of Problem \((\text{SVM}_{s_2'})\) with \( w \neq 0 \) and \( \eta > 0 \), and if \( 2/(p+q) \leq \nu < 4/(p+q) \) and \( p_f, q_f \geq 2 \), then \( \eta \) and \( b \) can always be determined from an optimal solution \( (\lambda, \mu) \) of the dual.

**Proof.** Since \( p_f + q_f \geq 4 \), by Proposition 34.5, either there is some \( i_0 \) such that \( \epsilon_{i_0} = 0 \) and the constraint \( w^\top u_{i_0} - b = \eta \) is active, or there is some \( j_0 \) such that \( \xi_{j_0} = 0 \) and the constraint \( -w^\top v_{j_0} + b = \eta \) is active. As we already explained, Problem \((\text{SVM}_{s_2'})\) satisfies the conditions for having a zero duality gap. Therefore, for optimal solutions we have

\[
L(w, \epsilon, \xi, b, \eta, \lambda, \mu, \alpha, \beta) = G(\lambda, \mu, \alpha, \beta),
\]

which means that

\[
\frac{1}{2} w^\top w - \nu \eta + \frac{1}{p+q} \left( \sum_{i=1}^{p} \epsilon_i + \sum_{j=1}^{q} \xi_j \right) = -\frac{1}{2} (\lambda^\top \mu^\top) X^\top X \left( \begin{array}{c} \lambda \\ \mu \end{array} \right),
\]

and since

\[
w = -X \left( \begin{array}{c} \lambda \\ \mu \end{array} \right),
\]

we get

\[
\frac{1}{p+q} \left( \sum_{i=1}^{p} \epsilon_i + \sum_{j=1}^{q} \xi_j \right) = \nu \eta - (\lambda^\top \mu^\top) X^\top X \left( \begin{array}{c} \lambda \\ \mu \end{array} \right). \tag{\ast}
\]

Let \( I = \{i \in \{1, \ldots, p\} \mid \epsilon_i > 0\} \) and \( J = \{j \in \{1, \ldots, q\} \mid \xi_j > 0\} \). By hypothesis \(|I| \geq 2\) and \(|J| \geq 2\). We know that \( \lambda_i = 1/(p+q) \) for all \( i \in I \) and \( \mu_j = 1/(p+q) \) for all \( j \in J \), so the following equations are active:

\[
w^\top u_i - b = \eta - \epsilon_i \quad i \in I
\]

\[-w^\top v_j + b = \eta - \xi_j \quad j \in J.
\]

But \((\ast)\) can be written as

\[
\frac{1}{p+q} \left( \sum_{i \in I} \epsilon_i + \sum_{j \in J} \xi_j \right) = \nu \eta - (\lambda^\top \mu^\top) X^\top X \left( \begin{array}{c} \lambda \\ \mu \end{array} \right), \tag{\ast\ast}
\]
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and since
\[ \epsilon_i = \eta - w^T u_i + b \quad i \in I \]
\[ \xi_j = \eta + w^T v_j - b \quad j \in J. \]

by substituting in the equation (**) we get

\[ \left( \frac{|I| + |J|}{p + q} - \nu \right) \eta = \frac{|J| - |I| b}{p + q} + \frac{1}{p + q} w^T \left( \sum_{i \in I} u_i - \sum_{j \in J} v_j \right) - \left( \lambda^T \mu^T \right) X^T X \left( \lambda \mu \right). \]

We also know that either \( w^T u_{i_0} - b = \eta \) or \( -w^T v_{j_0} + b = \eta \). In the first case, \( b = -\eta + w^T u_{i_0} \), and by substituting \( b \) in the above equation we get an equation of the form

\[ \left( \frac{|I| + |J|}{p + q} - \nu \right) \eta = -\frac{|J| - |I|}{p + q} \eta + T_1, \]

that is,

\[ \left( \frac{2|J|}{p + q} - \nu \right) \eta = T_1. \]

In the second case \( b = \eta + w^T v_{j_0} \), and we get an equation of the form

\[ \left( \frac{|I| + |J|}{p + q} - \nu \right) \eta = \frac{|J| - |I|}{p + q} \eta + T_2, \]

that is,

\[ \left( \frac{2|I|}{p + q} - \nu \right) \eta = T_2. \]

We need to choose \( \nu \) such that \( 2|I|/(p + q)| - \nu \neq 0 \) and \( 2|J|/(p + q) - \nu \neq 0 \). Since \( |I| \geq 2 \) and \( |J| \geq 2 \), this will be the case if \( \nu < 4/(p + q) \). If this condition is satisfied we can solve for \( \eta \), and then we find \( b \) from either \( b = -\eta + w^T u_{i_0} \) or \( b = \eta + w^T v_{j_0} \).

Remark: If the the sets \( \{u_i\} \) and \( \{v_j\} \) are linearly separable, then we know from Theorem 31.10 that some \( u_i \) is on the blue margin and some \( v_j \) is on the red margin, so \( b \) and \( \delta \) can be determined. Although we can ensure that some \( u_i \) is classified correctly or some \( v_j \) is classified correctly, it does not seem possible to prove that the corresponding constraints are active without additional hypotheses (such as \( p_f + q_f \geq 3 \)).

Among its advantages, the support vector machinery is conducive to finding interesting statistical bounds in terms of the VC dimension, a notion invented by Vapnik and Chernovenkis. We will not go into this here and instead refer the reader to Vapnik [111] (especially, Chapter 4 and Chapters 9-13).

The “kernelized” version of Problem (SVMs2) is the following:
Soft margin kernel SVM (SVM$_{s2'}$):

\[
\begin{align*}
\text{minimize} & \quad \frac{1}{2}\langle w, w \rangle - \nu \eta + \frac{1}{p + q} \left( \epsilon^T \xi^T \right) 1_{p+q} \\
\text{subject to} & \quad \langle w, \phi(u_i) \rangle - b \geq \eta - \epsilon_i, \quad \epsilon_i \geq 0 \quad i = 1, \ldots, p \\
& \quad -\langle w, \phi(v_j) \rangle + b \geq \eta - \xi_j, \quad \xi_j \geq 0 \quad j = 1, \ldots, q \\
& \quad \eta \geq 0.
\end{align*}
\]

Tracing through the derivation of the dual program, we obtain

\[
\begin{align*}
\text{minimize} & \quad \frac{1}{2} \langle \lambda^T \mu^T \rangle K \left( \lambda \mu \right) \\
\text{subject to} & \quad \sum_{i=1}^{p} \lambda_i = \sum_{j=1}^{q} \mu_j \\
& \quad \lambda_i + \sum_{j=1}^{q} \mu_j \geq K_m \\
& \quad 0 \leq \lambda_i \leq K_s, \quad i = 1, \ldots, p \\
& \quad 0 \leq \mu_j \leq K_s, \quad j = 1, \ldots, q,
\end{align*}
\]

where $K$ is the kernel matrix of Section 34.1.

As in Section 34.2, we obtain

\[
w = \sum_{i=1}^{p} \lambda_i \phi(u_i) - \sum_{j=1}^{q} \mu_j \phi(v_j),
\]

so

\[
b = \frac{1}{2} \left( \sum_{i=1}^{p} \lambda_i \kappa(u_i, u_{i0}) + \kappa(u_i, v_{j0})\right) - \sum_{j=1}^{q} \mu_j \left( \kappa(v_j, u_{i0}) + \kappa(v_j, v_{j0}) \right)
\]

and the classification function

\[
f(x) = \text{sgn}(\langle w, \phi(x) \rangle - b)
\]

is given by

\[
f(x) = \text{sgn} \left( \sum_{i=1}^{p} \lambda_i (2\kappa(u_i, x) - \kappa(u_i, u_{i0}) - \kappa(u_i, v_{j0})) \\
- \sum_{j=1}^{q} \mu_j (2\kappa(v_j, x) - \kappa(v_j, u_{i0}) - \kappa(v_j, v_{j0}))) \right).
\]
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17.4 Soft Margin SVM; \((\text{SVM}_{s3})\)

In this section we consider the version of Problem \((\text{SVM}_{s2'})\) in which instead of using the function \(K\left(\sum_{i=1}^{p} \epsilon_i + \sum_{j=1}^{q} \xi_j\right)\) as a regularizing function we use the quadratic function \(K(\|\epsilon\|_2^2 + \|\xi\|_2^2)\).

**Soft margin SVM \((\text{SVM}_{s3})\):**

\[
\begin{align*}
\text{minimize} \ & \frac{1}{2} w^\top w - \nu \eta + K(\epsilon^\top \epsilon + \xi^\top \xi) \\
\text{subject to} \ & \quad w^\top u_i - b \geq \eta - \epsilon_i, \quad i = 1, \ldots, p \\
& \quad -w^\top v_j + b \geq \eta - \xi_j, \quad j = 1, \ldots, q \\
& \quad \eta \geq 0,
\end{align*}
\]

where \(\nu\) and \(K\) are two given positive constants. As we saw earlier, it is convenient to pick \(K = 1/(p+q)\).

The new twist with this formulation of the problem is that if \(\epsilon_i < 0\), then the corresponding inequality \(w^\top u_i - b \geq \eta - \epsilon_i\) implies the inequality \(w^\top u_i - b \geq \eta\) obtained by setting \(\epsilon_i\) to zero while reducing the value of \(\|\epsilon\|^2\), and similarly if \(\xi_j < 0\), then the corresponding inequality \(-w^\top v_j + b \geq \eta - \xi_j\) implies the inequality \(-w^\top v_j + b \geq \eta\) obtained by setting \(\xi_j\) to zero while reducing the value of \(\|\xi\|^2\). Therefore, if \((w, b, \epsilon, \xi)\) is an optimal solution of Problem \((\text{SVM}_{s3})\) it is not necessary to restrict the slack variables \(\epsilon_i\) and \(\xi_j\) to the nonnegative, which simplifies matters a bit.

One of the advantages of this methods is that \(\epsilon\) is determined by \(\lambda\) and \(\xi\) is determined by \(\mu\). We could also omit the constraint \(\eta \geq 0\), because for an optimal solution it can be shown using duality that \(\eta \geq 0\).

The Lagrangian is given by

\[
L(w, \epsilon, \xi, b, \eta, \lambda, \mu, \gamma) = \frac{1}{2} w^\top w - \nu \eta + K(\epsilon^\top \epsilon + \xi^\top \xi) + w^\top X \begin{pmatrix} \lambda \\ \mu \end{pmatrix} + \epsilon^\top \lambda - \xi^\top \mu + b(1_p^\top \lambda - 1_q^\top \mu) + \eta(1_p^\top \lambda + 1_q^\top \mu) - \gamma \eta
\]

\[
= \frac{1}{2} w^\top w + \epsilon^\top \lambda + 1_p^\top \lambda - \nu - \gamma
\]

\[
+ K(\epsilon^\top \epsilon + \xi^\top \xi) - \epsilon^\top \lambda - \xi^\top \mu + b(1_p^\top \lambda - 1_q^\top \mu).
\]

To find the dual function \(G(\lambda, \mu, \gamma)\) we minimize \(L(w, \epsilon, \xi, b, \eta, \lambda, \mu, \gamma)\) with respect to \(w, \epsilon, \xi, b, \) and \(\eta\). Since the Lagrangian is convex and \((w, \epsilon, \xi, b, \eta) \in \mathbb{R}^n \times \mathbb{R}^p \times \mathbb{R}^q \times \mathbb{R} \times \mathbb{R}\), a convex open set, by Theorem 21.11, the Lagrangian has a minimum in \((w, \epsilon, \xi, b, \eta)\) iff \(\nabla L_{w,\epsilon,\xi,b,\eta} = 0\),
so we compute $\nabla L_{w,\epsilon,\xi,b,\eta}$. The gradient $\nabla L_{w,\epsilon,\xi,b,\eta}$ is given by

$$
\nabla L_{w,\epsilon,\xi,b,\eta} = 
\begin{pmatrix}
w + X \left( \begin{array}{c} \lambda \\ \mu \end{array} \right) \\
2K\epsilon - \lambda \\
2K\xi - \mu \\
1_p^T \lambda - 1_q^T \mu \\
1_p^T \lambda + 1_q^T \mu - \nu - \gamma
\end{pmatrix}
$$

By setting $\nabla L_{w,\epsilon,\xi,b,\eta} = 0$ we get the equations

$$w = -X \left( \begin{array}{c} \lambda \\ \mu \end{array} \right) \quad (*)_w$$

and

$$
2K\epsilon = \lambda \\
2K\xi = \mu \\
1_p^T \lambda = 1_q^T \mu \\
1_p^T \lambda + 1_q^T \mu = \nu + \gamma.
$$

The last two equations are identical to the last two equations obtained in Problem (SVMs2'). We can use the other equations to obtain the following expression for the dual function $G(\lambda, \mu, \gamma)$,

$$
G(\lambda, \mu, \gamma) = -\frac{1}{4K}(\lambda^T \lambda + \mu^T \mu) - \frac{1}{2}(\lambda^T \mu^T) X^T X \left( \begin{array}{c} \lambda \\ \mu \end{array} \right) \\
= -\frac{1}{2}(\lambda^T \mu^T) \left( X^T X + \frac{1}{2K}I_{p+q} \right) \left( \begin{array}{c} \lambda \\ \mu \end{array} \right).
$$

Consequently the dual program is equivalent to the minimization program

$$
\text{minimize} \quad \frac{1}{2}(\lambda^T \mu^T) \left( X^T X + \frac{1}{2K}I_{p+q} \right) \left( \begin{array}{c} \lambda \\ \mu \end{array} \right)
$$

subject to

$$
\sum_{i=1}^p \lambda_i = \sum_{j=1}^q \mu_j
$$

$$
\sum_{i=1}^p \lambda_i + \sum_{j=1}^q \mu_j \geq \nu
$$

$$
\lambda_i \geq 0, \quad i = 1, \ldots, p
$$

$$
\mu_j \geq 0, \quad j = 1, \ldots, q.
$$
The above program is similar to the program that was obtained for Problem (SVMs₂') but the matrix $X^\top X$ is replaced by the matrix $X^\top X + (1/2K)I_{p+q}$, which is positive definite since $K > 0$, and also the inequalities $\lambda_i \leq K$ and $\mu_j \leq K$ no longer hold. However, the constraints imply that there is some $i_0$ such that $\lambda_{i_0} > 0$ and some $j_0$ such that $\mu_{j_0} > 0$.

The dual program is solved by making use of numerical procedures based on gradient descent. If the primal problem is solvable, this yields solutions for $\lambda$ and $\mu$. We obtain $w$ from $\lambda$ and $\mu$, and $\gamma$, as in Problem (SVMs₂'); namely,

$$w = \sum_{i=1}^{p} \lambda_i u_i - \sum_{j=1}^{q} \mu_j v_j.$$

Since the variables $\epsilon_i$ and $\mu_j$ are not restricted to be nonnegative we no longer have complementary slackness conditions involving them, but we know that

$$\epsilon = \frac{\lambda}{2K}, \quad \xi = \frac{\mu}{2K}.$$ 

Also since the constraints

$$\sum_{i=1}^{p} \lambda_i \geq \frac{\nu}{2} \quad \text{and} \quad \sum_{j=1}^{q} \mu_j \geq \frac{\nu}{2}$$

imply that there is some $i_0$ such that $\lambda_{i_0} > 0$ and some $j_0$ such that $\mu_{j_0} > 0$, we have $\epsilon_{i_0} > 0$ and $\xi_{j_0} > 0$, which means that at least two points are misclassified, so Problem (SVMs₃) should only be used when the sets $\{u_i\}$ and $\{v_j\}$ are not linearly separable. We can solve for $b$ and $\eta$ using the active constraints corresponding to any $i_0$ such that $\lambda_{i_0} > 0$ and any $j_0$ such that $\mu_{j_0} > 0$ and we get

$$b = \frac{w^\top u_{i_0} + w^\top v_{j_0}}{2},$$

$$\eta = \frac{w^\top u_{i_0} - w^\top v_{j_0}}{2}.$$

We can also use the fact that the optimality gap is 0 to find $\eta$. We have

$$\frac{1}{2} w^\top w - \nu \eta + K(\epsilon^\top \epsilon + \xi^\top \xi) = -\frac{1}{2} \left( \begin{array}{c} \lambda^\top \\ \mu^\top \end{array} \right)^\top \left( \begin{array}{c} X^\top X + \frac{1}{2K}I_{p+q} \\ 0 \end{array} \right) \left( \begin{array}{c} \lambda \\ \mu \end{array} \right),$$

and since

$$w = -X \left( \begin{array}{c} \lambda \\ \mu \end{array} \right)$$

we get

$$\nu \eta = K(\lambda^\top \lambda + \mu^\top \mu) + \left( \begin{array}{c} \lambda^\top \\ \mu^\top \end{array} \right)^\top \left( \begin{array}{c} X^\top X + \frac{1}{4K}I_{p+q} \\ 0 \end{array} \right) \left( \begin{array}{c} \lambda \\ \mu \end{array} \right).$$

The above confirms that at optimality we have $\eta \geq 0$. 
The “kernelized” version of Problem (SVM$_s^3$) is the following:

**Soft margin kernel SVM (SVM$_s^3$):**

\[
\begin{align*}
\text{minimize} & \quad \frac{1}{2} \langle w, w \rangle - \nu \eta + \frac{1}{p + q} (\epsilon^\top \epsilon + \xi^\top \xi) \\
\text{subject to} & \quad \langle w, \varphi(u_i) \rangle - b \geq \eta - \epsilon_i, \quad i = 1, \ldots, p \\
& \quad - \langle w, \varphi(v_j) \rangle + b \geq \eta - \xi_j, \quad j = 1, \ldots, q \\
& \quad \eta \geq 0.
\end{align*}
\]

By going over the derivation of the dual program, we obtain

\[
\begin{align*}
\text{minimize} & \quad \frac{1}{2} (\lambda^\top \mu^\top) (K + \frac{p + q}{2} I_{p+q}) (\lambda) \\
\text{subject to} & \quad \sum_{i=1}^{p} \lambda_i = \sum_{j=1}^{q} \mu_j \\
& \quad \sum_{i=1}^{p} \lambda_i + \sum_{j=1}^{q} \mu_j \geq \nu \\
& \quad \lambda_i \geq 0, \quad i = 1, \ldots, p \\
& \quad \mu_j \geq 0, \quad j = 1, \ldots, q,
\end{align*}
\]

where $K$ is the kernel matrix of Section 34.1. Then $w$, $b$, and $f(x)$ are obtained exactly as in Section 34.3.

### 17.5 Soft Margin Support Vector Machines; (SVM$_{s4}$)

In this section we consider a variation of Problem (SVM$_{s2'}$) by adding the term $(1/2)b^2$ to the objective function. The result is that in minimizing the Lagrangian to find the dual function $G$, not just $w$ but also $b$ is determined. We also suppress the constraint $\eta \geq 0$ which turns out to be redundant.

**Soft margin SVM (SVM$_{s4}$):**

\[
\begin{align*}
\text{minimize} & \quad \frac{1}{2} w^\top w + \frac{1}{2} b^2 + K \left( -\nu \eta + \frac{1}{p + q} (\epsilon^\top \xi^\top) 1_{p+q} \right) \\
\text{subject to} & \quad w^\top u_i - b \geq \eta - \epsilon_i, \quad \epsilon_i \geq 0 \quad i = 1, \ldots, p \\
& \quad - w^\top v_j + b \geq \eta - \xi_j, \quad \xi_j \geq 0 \quad j = 1, \ldots, q.
\end{align*}
\]
To simplify the presentation we assume that $K = 1$ and we write $K_s$ for $1/(p + q)$.

The Lagrangian $L(w, \epsilon, \xi, b, \eta, \lambda, \mu, \alpha, \beta)$ with $\lambda, \alpha \in \mathbb{R}^p_+$, $\mu, \beta \in \mathbb{R}^q_+$ is given by

$$L(w, \epsilon, \xi, b, \eta, \lambda, \mu, \alpha, \beta) = \frac{1}{2} w^\top w + w^\top X \begin{pmatrix} \lambda \\ \mu \end{pmatrix} + \frac{b^2}{2} - \nu \eta + K_s (\epsilon^\top \mathbf{1}_p + \xi^\top \mathbf{1}_q) - \epsilon^\top (\lambda + \alpha) - \xi^\top (\mu + \beta) + b (\mathbf{1}_p^\top \lambda - \mathbf{1}_q^\top \mu) + \eta (\mathbf{1}_p^\top \lambda + \mathbf{1}_q^\top \mu)$$

$$= \frac{1}{2} w^\top w + w^\top X \begin{pmatrix} \lambda \\ \mu \end{pmatrix} + \frac{b^2}{2} + b (\mathbf{1}_p^\top \lambda - \mathbf{1}_q^\top \mu) + \eta (\mathbf{1}_p^\top \lambda + \mathbf{1}_q^\top \mu - \nu) + \epsilon^\top (K_s \mathbf{1}_p - (\lambda + \alpha)) + \xi^\top (K_s \mathbf{1}_q - (\mu + \beta)).$$

To find the dual function $G(\lambda, \mu, \alpha, \beta)$, we minimize $L(w, \epsilon, \xi, b, \eta, \lambda, \mu, \alpha, \beta)$ with respect to $w, \epsilon, \xi, b, \eta$. Since the Lagrangian is convex and $(w, \epsilon, \xi, b, \eta) \in \mathbb{R}^n \times \mathbb{R}^p \times \mathbb{R}^q \times \mathbb{R} \times \mathbb{R}$, a convex open set, by Theorem 21.11, the Lagrangian has a minimum in $(w, \epsilon, \xi, b, \eta)$ iff $\nabla L_{w,\epsilon,\xi,b,\eta} = 0$, so we compute its gradient with respect to $w, \epsilon, \xi, b, \eta$ and we get

$$\nabla L_{w,\epsilon,\xi,b,\eta} = \begin{pmatrix} X \begin{pmatrix} \lambda \\ \mu \end{pmatrix} + w \\ K_s \mathbf{1}_p - (\lambda + \alpha) \\ K_s \mathbf{1}_q - (\mu + \beta) \\ b + \mathbf{1}_p^\top \lambda - \mathbf{1}_q^\top \mu \\ \mathbf{1}_p^\top \lambda + \mathbf{1}_q^\top \mu - \nu \end{pmatrix}.$$ 

By setting $\nabla L_{w,\epsilon,\xi,b,\eta} = 0$ we get the equations

$$w = -X \begin{pmatrix} \lambda \\ \mu \end{pmatrix} \quad \text{(**w)}$$

$$\lambda + \alpha = K_s \mathbf{1}_p$$

$$\mu + \beta = K_s \mathbf{1}_q$$

$$\mathbf{1}_p^\top \lambda + \mathbf{1}_q^\top \mu = \nu,$$

and

$$b = -(\mathbf{1}_p^\top \lambda - \mathbf{1}_q^\top \mu). \quad (**b)$$

The second and third equations are equivalent to the box constraints

$$0 \leq \lambda_i, \mu_j \leq K_s, \quad i = 1, \ldots, p, \quad j = 1, \ldots, q.$$

Since we assumed that the primal problem has an optimal solution with $w \neq 0$, we have

$$X \begin{pmatrix} \lambda \\ \mu \end{pmatrix} \neq 0.$$
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Plugging back $w$ from ($w$) and $b$ from ($b$) into the Lagrangian, we get
\[
G(\lambda, \mu, \alpha, \beta) = \frac{1}{2} (\lambda^\top \mu^\top) X^\top X \left(\begin{array}{c} \lambda \\ \mu \end{array}\right) - \frac{1}{2} (\lambda^\top \mu^\top) X^\top X \left(\begin{array}{c} \lambda \\ \mu \end{array}\right) + \frac{1}{2} b^2 - b^2
\]

\[
= -\frac{1}{2} (\lambda^\top \mu^\top) X^\top X \left(\begin{array}{c} \lambda \\ \mu \end{array}\right) - \frac{1}{2} b^2
\]

\[
= -\frac{1}{2} (\lambda^\top \mu^\top) \left( X^\top X + \begin{pmatrix} 1_p & 1_p^\top \\ -1_q & 1_q^\top \end{pmatrix} \begin{pmatrix} -1_p & 1_p^\top \\ 1_q & 1_q^\top \end{pmatrix} \right) \left(\begin{array}{c} \lambda \\ \mu \end{array}\right),
\]

so the dual function is independent of $\alpha, \beta$ and is given by
\[
G(\lambda, \mu) = -\frac{1}{2} (\lambda^\top \mu^\top) \left( X^\top X + \begin{pmatrix} 1_p & 1_p^\top \\ -1_q & 1_q^\top \end{pmatrix} \begin{pmatrix} -1_p & 1_p^\top \\ 1_q & 1_q^\top \end{pmatrix} \right) \left(\begin{array}{c} \lambda \\ \mu \end{array}\right).
\]

The dual program is given by
\[
\text{maximize} \quad -\frac{1}{2} (\lambda^\top \mu^\top) \left( X^\top X + \begin{pmatrix} 1_p & 1_p^\top \\ -1_q & 1_q^\top \end{pmatrix} \begin{pmatrix} -1_p & 1_p^\top \\ 1_q & 1_q^\top \end{pmatrix} \right) \left(\begin{array}{c} \lambda \\ \mu \end{array}\right)
\]

subject to
\[
\sum_{i=1}^p \lambda_i + \sum_{j=1}^q \mu_j = \nu
\]

\[
0 \leq \lambda_i \leq K_s, \quad i = 1, \ldots, p
\]

\[
0 \leq \mu_j \leq K_s, \quad j = 1, \ldots, q.
\]

Finally, the dual program is equivalent to the following minimization program:
\[
\text{minimize} \quad \frac{1}{2} (\lambda^\top \mu^\top) \left( X^\top X + \begin{pmatrix} 1_p & 1_p^\top \\ -1_q & 1_q^\top \end{pmatrix} \begin{pmatrix} -1_p & 1_p^\top \\ 1_q & 1_q^\top \end{pmatrix} \right) \left(\begin{array}{c} \lambda \\ \mu \end{array}\right)
\]

subject to
\[
\sum_{i=1}^p \lambda_i + \sum_{j=1}^q \mu_j = \nu
\]

\[
0 \leq \lambda_i \leq K_s, \quad i = 1, \ldots, p
\]

\[
0 \leq \mu_j \leq K_s, \quad j = 1, \ldots, q.
\]

The dual program is solved by making use of numerical procedures based on gradient descent. If the primal problem is solvable, this yields solutions for $\lambda$ and $\mu$. Once a solution for $\lambda$ and $\mu$ is obtained, we have
\[
w = -X \left(\begin{array}{c} \lambda \\ \mu \end{array}\right) = \sum_{i=1}^p \lambda_i u_i - \sum_{j=1}^q \mu_j v_j
\]

\[
b = -\sum_{i=1}^p \lambda_i + \sum_{j=1}^q \mu_j.
\]
As we said earlier, the hypotheses of Theorem 31.14(2) hold, so if the primal problem \((\text{SVM}_{s4})\) has an optimal solution with \(w \neq 0\), then the dual problem has a solution too, and the duality gap is zero. Therefore, for optimal solutions we have

\[
L(w, \epsilon, \xi, b, \eta, \lambda, \mu, \alpha, \beta) = G(\lambda, \mu, \alpha, \beta),
\]

which means that

\[
\frac{1}{2}w^\top w + \frac{b^2}{2} - \nu \eta + K_s \left( \sum_{i=1}^{p} \epsilon_i + \sum_{j=1}^{q} \xi_j \right) = -\frac{1}{2} \left( \lambda^\top \mu^\top \right) \left( X^\top X + \begin{pmatrix} \frac{1}{p} & -\frac{1}{q} \\ -\frac{1}{q} & \frac{1}{p} \end{pmatrix} \right) \left( \begin{pmatrix} \lambda \\ \mu \end{pmatrix} \right)
\]

and since

\[
\frac{1}{2}w^\top w + \frac{b^2}{2} = \frac{1}{2} \left( \lambda^\top \mu^\top \right) \left( X^\top X + \begin{pmatrix} \frac{1}{p} & -\frac{1}{q} \\ -\frac{1}{q} & \frac{1}{p} \end{pmatrix} \right) \left( \begin{pmatrix} \lambda \\ \mu \end{pmatrix} \right),
\]

we get

\[
\eta = K_s \nu \left( \sum_{i=1}^{p} \epsilon_i + \sum_{j=1}^{q} \xi_j \right) + \frac{1}{\nu} \left( \lambda^\top \mu^\top \right) \left( X^\top X + \begin{pmatrix} \frac{1}{p} & -\frac{1}{q} \\ -\frac{1}{q} & \frac{1}{p} \end{pmatrix} \right) \left( \begin{pmatrix} \lambda \\ \mu \end{pmatrix} \right).
\]

Since

\[
X^\top X + \begin{pmatrix} \frac{1}{p} & -\frac{1}{q} \\ -\frac{1}{q} & \frac{1}{p} \end{pmatrix}
\]

is positive semidefinite, so we confirm that \(\eta \geq 0\).

Since \(K_s = 1/(p + q)\), in order for the constraints

\[
\sum_{i=1}^{p} \lambda_i + \sum_{j=1}^{q} \mu_j = \nu
\]

and \(0 \leq \lambda_i, \mu_j \leq 1/(p + q)\) to be satisfied we must have

\[
\nu \leq 1.
\]

The equation

\[
\sum_{i=1}^{p} \lambda_i + \sum_{j=1}^{q} \mu_j = \nu
\]

also implies that either there is some \(i_0\) such that \(\lambda_{i_0} > 0\) or there is some \(j_0\) such that \(\mu_{j_0} > 0\).

Under the **Standard Margin Hypothesis** for \((\text{SVM}_{s4})\), either there is some \(i_0\) such that \(0 < \lambda_{i_0} < K_s\) or there is some \(j_0\) such that \(0 < \mu_{j_0} < K_s\), and by the complementary slackness conditions \(\epsilon_{i_0} = 0\) or \(\xi_{j_0} = 0\), so we have

\[
w^\top u_{i_0} - b = \eta, \quad \text{or} \quad -w^\top v_{j_0} + b = \eta,
\]
and we can solve for $\eta$.

The equations (†) and the box inequalities
\[ 0 \leq \lambda_i \leq K_s, \quad 0 \leq \mu_j \leq K_s \]
also imply the following facts:

**Proposition 17.4.** If Problem $(\text{SVM}_{s4})$ has an optimal solution with $w \neq 0$ and $\eta > 0$ then the following facts hold:

1. At most $\nu(p+q)$ points $u_i$ and $v_j$ fail to achieve the margin $\eta$.
2. At least $\nu(p+q)$ points $u_i$ and $v_j$ have margin at most $\eta$.

**Proof.** (1) Recall that for an optimal solution with $w \neq 0$ and $\eta > 0$ we have the equation
\[ \sum_{i=1}^{p} \lambda_i + \sum_{j=1}^{q} \mu_j = \nu. \]
If $u_i$ fails to achieve the margin $\eta$, then $\epsilon_i > 0$, and by complementary slackness $\lambda_i = K_s = 1/(p+q)$. Similarly, if $v_j$ fails to achieve the margin then $\xi_j > 0$, and by complementary slackness $\mu_j = K_s = 1/(p+q)$. Assume that $p_f$ points $u_i$ fail the margin and that $q_f$ points $v_j$ fail the margin. Then
\[ \nu = \sum_{i=1}^{p} \lambda_i + \sum_{j=1}^{q} \mu_j \geq p_f + q_f, \]
so
\[ p_f + q_f \leq \nu(p+q). \]

(2) A point $u_i$ has margin at most $\eta$ iff $\lambda_i > 0$ and a point $v_j$ has margin at most $\eta$ iff $\mu_j > 0$. If
\[ I_m = \{ i \in \{1, \ldots, p\} \mid \lambda_i > 0 \} \quad \text{and} \quad p_m = |I_m| \]
and
\[ J_m = \{ j \in \{1, \ldots, q\} \mid \mu_j > 0 \} \quad \text{and} \quad q_m = |J_m| \]
then
\[ \nu = \sum_{i=1}^{p} \lambda_i + \sum_{j=1}^{q} \mu_j = \sum_{i \in I_m} \lambda_i + \sum_{j \in J_m} \mu_j, \]
and since $\lambda_i, \mu_j \leq K_s = 1/(p+q)$, we have
\[ \nu = \sum_{i \in I_m} \lambda_i + \sum_{j \in J_m} \mu_j \leq \frac{p_m + q_m}{p+q}, \]
which yields
\[ p_m + q_m \geq \nu(p+q). \]

Note that if $\nu$ is chosen so that $\nu < 1/(p + q)$, then $\nu(p + q) < 1$, which means that none of the data points are misclassified; in other words, the $u_i$s and $v_j$s are linearly separable. Thus we see that if the $u_i$s and $v_j$s are not linearly separable we must pick $\nu$ such that $1/(p + q) \leq \nu \leq 1$ for the method to succeed.

The following proposition clarifies the role of the constant $\nu$ in establishing the trade-off between the width of the margin and the number of margin-error points. In particular, it shows that if Problem (SVM$_{ad}$) has an optimal solution with $w \neq 0$ and $\eta > 0$, and if $\nu < 1$, then at least some $u_i$ or some $v_j$ is classified correctly. Obviously we have $1/(p + q) \leq 1$.

**Proposition 17.5.** Suppose $(w, b, \eta, \epsilon, \xi)$ is an optimal solution of Problem (SVM$_{ad}$) with $w \neq 0$ and $\eta > 0$, and let $p_f$ be the number of points $u_i$ that are misclassified ($\epsilon_i > 0$) and $q_f$ be the number of points $v_j$ that are misclassified ($\xi_j > 0$). If $p_f + q_f \geq 2$ and if $1/(p + q) \leq \nu < (p_f + q_f)/(p + q)$, then either there is some $i$ such that $\epsilon_i = 0$ and the constraint $w^\top u_i - b = \eta$ is active, or there is some $j$ such that $\xi_j = 0$ and the constraint $-w^\top v_j + b = \eta$ is active.

**Proof.** (1) We may assume that $K_s = 1/(p + q)$. We proceed by contradiction. Thus we assume that for all $i \in \{1, \ldots, p\}$, if $\epsilon_i = 0$ then the constraint $w^\top u_i - b \geq \eta$ is not active, namely $w^\top u_i - b > \eta$, and for all $j \in \{1, \ldots, q\}$, if $\xi_j = 0$ then the constraint $-w^\top v_j + b \geq \eta$ is not active, namely $-w^\top v_j + b > \eta$.

Let $I = \{i \in \{1, \ldots, p\} \mid \epsilon_i > 0\}$, let $J = \{j \in \{1, \ldots, q\} \mid \xi_j > 0\}$, and let $p_f = |I|$ and $q_f = |J|$ (of course, $\eta > 0$).

Assume that $p_f + q_f \geq 2$. By complementary slackness all the constraints for which $i \in I$ and $j \in J$ are active, so our hypotheses are

\[
\begin{align*}
  w^\top u_i - b &= \eta - \epsilon_i & \epsilon_i > 0 & i \in I \\
  -w^\top v_j + b &= \eta - \xi_j & \xi_j > 0 & j \in J \\
  w^\top u_i - b &> \eta & i \notin I \\
  -w^\top v_j + b &> \eta & j \notin J.
\end{align*}
\]

For any $\theta > 0$ such that

\[
\theta < \min\{\epsilon_i, \xi_j, \eta \mid i \in \{1, \ldots, p\}, j \in \{1, \ldots, q\}\},
\]

we can write

\[
\begin{align*}
  w^\top u_i - b &= \eta - \theta - (\epsilon_i - \theta) & \epsilon_i - \theta \geq 0 & i \in I \\
  -w^\top v_j + b &= \eta - \theta - (\xi_j - \theta) & \xi_j - \theta \geq 0 & j \in J \\
  w^\top u_i - b &> \eta - \theta & i \notin I \\
  -w^\top v_j + b &> \eta - \theta & j \notin J.
\end{align*}
\]
The original value of the objective function is

\[ \omega(0) = \frac{1}{2} w^\top w - \nu \eta + \frac{1}{p + q} \left( \sum_{i \in I} \epsilon_i + \sum_{j \in J} \xi_j \right), \]

and the new value is

\[ \omega(\theta) = \frac{1}{2} w^\top w - \nu (\eta - \theta) + \frac{1}{p + q} \left( \sum_{i \in I} (\epsilon_i - \theta) + \sum_{j \in J} (\xi_j - \theta) \right) \]

\[ = \frac{1}{2} w^\top w - \nu \eta + \frac{1}{p + q} \left( \sum_{i \in I} \epsilon_i + \sum_{j \in J} \xi_j \right) - \left( \frac{p_f + q_f}{p + q} - \nu \right) \theta. \]

Since by hypothesis \( p_f + q_f \geq 2 \), if

\[ \frac{1}{p + 1} \leq \nu < \frac{p_f + q_f}{p + q}, \]

then the term involving \( \theta \) is negative so

\[ \omega(\theta) < \omega(0), \]

and by the choice of \( \theta \) we have \( \eta - \theta > 0 \), so \((w, b, \eta - \theta, \epsilon - \theta, \xi - \theta)\) is a feasible solution, contradicting the optimality of the solution \((w, b, \eta, \epsilon, \xi)\); here we write \( \epsilon - \theta \) for the vector \((\epsilon_1 - \theta, \ldots, \epsilon_p - \theta)\), and similarly for \( \xi - \theta \).

Note that if \( p_f + q_f = p + q \) and \( \nu < 1 \), then Proposition 34.5 yields a contradiction. Therefore \( p_f + q_f < p + q \), that is, at least some \( u_i \) or some \( v_j \) is classified correctly.

**Remark:** If the the sets \( \{u_i\} \) and \( \{v_j\} \) are linearly separable, then we know from Theorem 31.10 that some \( u_i \) is on the blue margin and some \( v_j \) is on the red margin.

We also have the following proposition that gives a sufficient condition implying that \( \eta \) can be found in terms of an optimal solution \((\lambda, \mu)\) of the dual.

**Proposition 17.6.** If \((w, b, \eta, \epsilon, \xi)\) is an optimal solution of Problem (SVM\(_{sa}\)) with \( w \neq 0 \) and \( \eta > 0 \), if \( 1/(p + q) \leq \nu < 2/(p + q) \) and \( p_f + q_f \geq 2 \), then \( \eta \) can always be determined from an optimal solution \((\lambda, \mu)\) of the dual.

**Proof.** As we already explained, Problem (SVM\(_{sa}\)) satisfies the conditions for having a zero duality gap. Therefore, for optimal solutions we have

\[ L(w, \epsilon, \xi, b, \eta, \lambda, \mu, \alpha, \beta) = G(\lambda, \mu, \alpha, \beta), \]

which means that

\[ \nu \eta = \frac{1}{p + q} \left( \sum_{i=1}^{p} \epsilon_i + \sum_{j=1}^{q} \xi_j \right) + (\lambda^\top \mu^\top) \left( X^\top X + \begin{pmatrix} \frac{1}{p}1_p^\top & -\frac{1}{p}1_q^\top \\ -\frac{1}{q}1_p^\top & \frac{1}{q}1_q^\top \end{pmatrix} \right) \left( \begin{array}{c} \lambda \\ \mu \end{array} \right). \]  \( \ast \)
Let \( I = \{i \in \{1, \ldots, p\} \mid \epsilon_i > 0\} \) and \( J = \{j \in \{1, \ldots, q\} \mid \zeta_j > 0\} \). If \( I = J = \emptyset \), then
\[
\eta = (\lambda^\top \mu^\top) \left( X^\top X + \begin{pmatrix} 1_p^\top 1_p^\top & -1_p^\top 1_q^\top \\ -1_q^\top 1_p^\top & 1_q^\top 1_q^\top \end{pmatrix} \right) \left( \lambda \right).
\]

Assume that \( |I| + |J| \geq 2 \). Then we know that \( \lambda_i = 1/(p+q) \) for all \( i \in I \) and \( \mu_j = 1/(p+q) \) for all \( j \in J \), so the following equations are active:
\[
\begin{align*}
    w^\top u_i - b &= \eta - \epsilon_i & i & \in I \\
    -w^\top v_j + b &= \eta - \zeta_j & j & \in J.
\end{align*}
\]
But (*) can be written as
\[
\nu \eta = \frac{1}{p+q} \left( \sum_{i \in I} \epsilon_i + \sum_{j \in J} \zeta_j \right) + (\lambda^\top \mu^\top) \left( X^\top X + \begin{pmatrix} 1_p^\top 1_p^\top & -1_p^\top 1_q^\top \\ -1_q^\top 1_p^\top & 1_q^\top 1_q^\top \end{pmatrix} \right) \left( \lambda \right),
\]
and since
\[
\begin{align*}
    \epsilon_i &= \eta - w^\top u_i + b & i & \in I \\
    \zeta_j &= \eta + w^\top v_j - b & j & \in J,
\end{align*}
\]
by substituting in the equation (**) we get
\[
\left( \frac{|I| + |J|}{p+q} - \nu \right) \eta = \frac{|J| - |I|}{p+q} b + \frac{1}{p+q} w^\top \left( \sum_{i \in I} u_i - \sum_{j \in J} v_j \right)
\]
\[
- (\lambda^\top \mu^\top) \left( X^\top X + \begin{pmatrix} 1_p^\top 1_p^\top & -1_p^\top 1_q^\top \\ -1_q^\top 1_p^\top & 1_q^\top 1_q^\top \end{pmatrix} \right) \left( \lambda \right).
\]
We need to choose \( \nu \) such that \( (|I| + |J|)/(p+q) - \nu \neq 0 \) Since we are assuming that \( |I| + |J| \geq 2 \), this will be the case if \( 1/(p+q) \leq \nu < 2/(p+q) \). If this condition is satisfied we can solve for \( \eta \).

\[\square\]

**Remark:** If the the sets \( \{u_i\} \) and \( \{v_j\} \) are linearly separable, then we know from Theorem 31.10 that some \( u_i \) is on the blue margin and some \( v_j \) is on the red margin, so \( b \) and \( \delta \) can be determined. Although we can ensure that some \( u_i \) is classified correctly or some \( v_j \) is classified correctly, it does not seem possible to prove that the corresponding constraints are active without additional hypotheses (such as \( p_f + q_f \geq 2 \)).

The “kernelized” version of Problem (SVM\(_{s4}\)) is the following:

**Soft margin kernel SVM (SVM\(_{s4}\)):**
\[
\text{minimize } \frac{1}{2} \langle w, w \rangle + \frac{1}{2} b^2 - \nu \eta + \frac{1}{p+q} \left( \epsilon^\top \zeta^\top \right) 1_{p+q}
\]
subject to
\[
\begin{align*}
    \langle w, \varphi(u_i) \rangle - b & \geq \eta - \epsilon_i, & \epsilon_i & \geq 0 & i & = 1, \ldots, p \\
    - \langle w, \varphi(v_j) \rangle + b & \geq \eta - \zeta_j, & \zeta_j & \geq 0 & j & = 1, \ldots, q.
\end{align*}
\]
Tracing through the derivation of the dual program, we obtain

\[
\begin{align*}
\text{minimize} & \quad \frac{1}{2} (\lambda^\top \mu^\top) \left( K + \begin{pmatrix} 1_p 1_p^\top & -1_p 1_q^\top \\ -1_q 1_p^\top & 1_q 1_q^\top \end{pmatrix} \right) \left( \begin{array}{c} \lambda \\ \mu \end{array} \right) \\
\text{subject to} & \quad \sum_{i=1}^{p} \lambda_i + \sum_{j=1}^{q} \mu_j = \nu \\
& \quad 0 \leq \lambda_i \leq K_s, \quad i = 1, \ldots, p \\
& \quad 0 \leq \mu_j \leq K_s, \quad j = 1, \ldots, q,
\end{align*}
\]

where \( K \) is the kernel matrix of Section 34.1.

We obtain

\[
\begin{align*}
w &= \sum_{i=1}^{p} \lambda_i \varphi(u_i) - \sum_{j=1}^{q} \mu_j \varphi(v_j) \\
b &= - \sum_{i=1}^{p} \lambda_i + \sum_{j=1}^{q} \mu_j.
\end{align*}
\]

The classification function

\[
f(x) = \text{sgn}(\langle w, \varphi(x) \rangle - b)
\]

is given by

\[
f(x) = \text{sgn} \left( \sum_{i=1}^{p} \lambda_i (\kappa(u_i, x) + 1) - \sum_{j=1}^{q} \mu_j (\kappa(v_j, x) + 1) \right).
\]

17.6 Soft Margin SVM; \((\text{SVM}_{s5})\)

In this section we consider the version of Problem \((\text{SVM}_{s5})\) in which we add the term \((1/2)b^2\) to the objective function. We also drop the constraint \(\eta \geq 0\) which is redundant.

Soft margin SVM \((\text{SVM}_{s5})\):

\[
\begin{align*}
\text{minimize} & \quad \frac{1}{2} w^\top w + \frac{1}{2} b^2 - \nu \eta + K(\epsilon^\top \epsilon + \xi^\top \xi) \\
\text{subject to} & \quad w^\top u_i - b \geq \eta - \epsilon_i, \quad i = 1, \ldots, p \\
& \quad -w^\top v_j + b \geq \eta - \xi_j, \quad j = 1, \ldots, q,
\end{align*}
\]
where $\nu$ and $K$ are two given positive constants. As we saw earlier, it is convenient to pick
$K = 1/(p + q)$.

The Lagrangian is given by

$$L(w, \epsilon, \xi, b, \eta, \lambda, \mu) = \frac{1}{2}w^\top w + \frac{1}{2}b^2 - \nu\eta + K(\epsilon^\top \epsilon + \xi^\top \xi) + w^\top X\begin{pmatrix} \lambda \\ \mu \end{pmatrix}
- \epsilon^\top \lambda - \xi^\top \mu + b(1_p^\top \lambda - 1_q^\top \mu) + \eta(1_p^\top \lambda + 1_q^\top \mu)
= \frac{1}{2}w^\top w + w^\top X\begin{pmatrix} \lambda \\ \mu \end{pmatrix} + \eta(1_p^\top \lambda + 1_q^\top \mu)
+ K(\epsilon^\top \epsilon + \xi^\top \xi) - \epsilon^\top \lambda - \xi^\top \mu + b(1_p^\top \lambda - 1_q^\top \mu) + \frac{1}{2}b^2.$$  

To find the dual function $G(\lambda, \mu)$ we minimize $L(w, \epsilon, \xi, b, \eta, \lambda, \mu)$ with respect to $w, \epsilon, \xi, b, \eta$. Since the Lagrangian is convex and $(w, \epsilon, \xi, b, \eta) \in \mathbb{R}^n \times \mathbb{R}^p \times \mathbb{R}^q \times \mathbb{R} \times \mathbb{R}$, a convex open set, by Theorem 21.11, the Lagrangian has a minimum in $(w, \epsilon, \xi, b, \eta)$ iff $\nabla L(w, \epsilon, \xi, b, \eta) = 0$, so we compute $\nabla L(w, \epsilon, \xi, b, \eta)$. The gradient $\nabla L(w, \epsilon, \xi, b, \eta)$ is given by

$$\nabla L(w, \epsilon, \xi, b, \eta) = \begin{pmatrix}
w + X\begin{pmatrix} \lambda \\ \mu \end{pmatrix}
2K\epsilon - \lambda
2K\xi - \mu
b + 1_p^\top \lambda - 1_q^\top \mu
1_p^\top \lambda + 1_q^\top \mu - \nu
\end{pmatrix}.$$  

By setting $\nabla L(w, \epsilon, \xi, b, \eta) = 0$ we get the equations

$$w = -X\begin{pmatrix} \lambda \\ \mu \end{pmatrix} \quad \text{(**w)}$$  

and

$$2K\epsilon = \lambda$$
$$2K\xi = \mu$$
$$b = -(1_p^\top \lambda - 1_q^\top \mu)$$
$$1_p^\top \lambda + 1_q^\top \mu = \nu.$$  

The last two equations are identical to the last two equations obtained in Problem (SVM_s4). We can use the other equations to obtain the following expression for the dual function $G(\lambda, \mu, \gamma)$,

$$G(\lambda, \mu, \gamma) = -\frac{1}{4K}(\lambda^\top \lambda + \mu^\top \mu) - \frac{1}{2}(\lambda^\top \mu) X^\top X\begin{pmatrix} \lambda \\ \mu \end{pmatrix} - \frac{b^2}{2}
= -\frac{1}{2}(\lambda^\top \mu) \left( X^\top X + \begin{pmatrix} 1_p & 1_p^\top \\ -1_q & 1_q^\top \\ 1_q & 1_q^\top 
\end{pmatrix} + \frac{1}{2K}I_{p+q} \right) \begin{pmatrix} \lambda \\ \mu \end{pmatrix}.$$  


Consequently the dual program is equivalent to the minimization program

\[
\text{minimize } \frac{1}{2} \begin{pmatrix} \lambda^T & \mu^T \end{pmatrix} \begin{pmatrix} X^T X + \left( \begin{array}{cc} 1_p & 1_p^T \\ -1_q 1_p & -1_q 1_q^T \end{array} \right) + \frac{1}{2K} I_{p+q} \end{pmatrix} \begin{pmatrix} \lambda \\ \mu \end{pmatrix},
\]

subject to

\[
\sum_{i=1}^p \lambda_i + \sum_{j=1}^q \mu_j = \nu \\
\lambda_i \geq 0, \quad i = 1, \ldots, p \\
\mu_j \geq 0, \quad j = 1, \ldots, q.
\]

The dual program is solved by making use of numerical procedures based on gradient descent. If the primal problem is solvable, this yields solutions for \( \lambda \) and \( \mu \).

The constraints imply that either there is some \( i_0 \) such that \( \lambda_{i_0} > 0 \) or there is some \( j_0 \) such that \( \mu_{j_0} > 0 \). We obtain \( w \) and \( b \) from \( \lambda \) and \( \mu \), as in Problem (SVM\(_{s4}\)); namely,

\[
w = \sum_{i=1}^p \lambda_i u_i - \sum_{j=1}^q \mu_j v_j \\
b = -\sum_{i=1}^p \lambda_i + \sum_{j=1}^q \mu_j.
\]

Since the variables \( \epsilon_i \) and \( \mu_j \) are not restricted to be nonnegative we no longer have complementary slackness conditions involving them, but we know that

\[
\epsilon = \frac{\lambda}{2K}, \quad \xi = \frac{\mu}{2K}.
\]

Also since the constraint

\[
\sum_{i=1}^p \lambda_i + \sum_{j=1}^q \mu_j = \nu
\]

implies that either there is some \( i_0 \) such that \( \lambda_{i_0} > 0 \) or there is some \( j_0 \) such that \( \mu_{j_0} > 0 \), we have \( \epsilon_{i_0} > 0 \) or \( \xi_{j_0} > 0 \), which means that at least one point is misclassified, so Problem (SVM\(_{s5}\)) should only be used when the sets \( \{u_i\} \) and \( \{v_j\} \) are not linearly separable. We can solve for \( \eta \) using the active constraints corresponding to any \( i_0 \) such that \( \lambda_{i_0} > 0 \) or any \( j_0 \) such that \( \mu_{j_0} > 0 \).

We can also use the fact that the optimality gap is 0 to find \( \eta \). We have

\[
\frac{1}{2} w^T w + \frac{b^2}{2} - \nu \eta + K(\epsilon^T \epsilon + \xi^T \xi) = \frac{1}{2} \begin{pmatrix} \lambda^T & \mu^T \end{pmatrix} \begin{pmatrix} X^T X + \left( \begin{array}{cc} 1_p & 1_p^T \\ -1_q 1_p & -1_q 1_q^T \end{array} \right) + \frac{1}{2K} I_{p+q} \end{pmatrix} \begin{pmatrix} \lambda \\ \mu \end{pmatrix},
\]

so we get

\[
\nu \eta = K(\lambda^T \lambda + \mu^T \mu) + (\lambda^T \mu^T) \begin{pmatrix} X^T X \left( \begin{array}{cc} 1_p & 1_p^T \\ -1_q 1_p & -1_q 1_q^T \end{array} \right) + \frac{1}{4K} I_{p+q} \end{pmatrix} \begin{pmatrix} \lambda \\ \mu \end{pmatrix}.
\]
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The above confirms that at optimality we have \( \eta \geq 0 \).

The “kernelized” version of Problem (SVMs) is the following:

**Soft margin kernel SVM (SVM_{s5}):**

\[
\begin{align*}
\text{minimize} & \quad \frac{1}{2} \langle w, w \rangle + \frac{1}{2} b^2 - \nu \eta + \frac{1}{p + q} (\epsilon^\top \epsilon + \xi^\top \xi) \\
\text{subject to} & \quad \langle w, \varphi(u_i) \rangle - b \geq \eta - \epsilon_i, \quad i = 1, \ldots, p \\
& \quad -\langle w, \varphi(v_j) \rangle + b \geq \eta - \xi_j, \quad j = 1, \ldots, q.
\end{align*}
\]

Tracing through the derivation of the dual program, we obtain

\[
\begin{align*}
\text{minimize} & \quad \frac{1}{2} \left( \lambda^\top \mu^\top \right) \left( K \right)
+ \left( \begin{array}{cc}
1_p & 1_p^\top \\
-1_q & 1_q^\top
\end{array} \right)
\left( \begin{array}{c}
p + q \\
2
\end{array} \right)
\left( \begin{array}{c}
\lambda \\
\mu
\end{array} \right) \\
\text{subject to} & \quad \sum_{i=1}^p \lambda_i + \sum_{j=1}^q \mu_j = \nu \\
& \quad \lambda_i \geq 0, \quad i = 1, \ldots, p \\
& \quad \mu_j \geq 0, \quad j = 1, \ldots, q,
\end{align*}
\]

where \( K \) is the kernel matrix of Section 34.1. Then \( w, b, \) and \( f(x) \) are obtained exactly as in Section 34.5.

### 17.7 Summary and Comparison of the SVM Methods

In this chapter we considered six variants for solving the soft margin binary classification problem for two sets of points \( \{u_i\}_{i=1}^p \) and \( \{v_j\}_{j=1}^q \) using support vector classification methods. The objective is to find a separating hyperplane \( H_{w,b} \) of equation \( w^\top x - b = 0 \). We also try to find two “margin hyperplanes” \( H_{w,b+\delta} \) of equation \( w^\top x - b - \delta = 0 \) and \( H_{w,b-\delta} \) of equation \( w^\top x - b + \delta = 0 \) such that \( \delta \) is as big as possible and yet the number of misclassified points is minimized, which is achieved by allowing an error \( \epsilon_i \geq 0 \) for every point \( u_i \), in the sense that the constraint

\[ w^\top u_i - b \geq \delta - \epsilon_i \]

should hold, and an error \( \xi_j \geq 0 \) for every point \( v_j \), in the sense that the constraint

\[ -w^\top v_j + b \geq \delta - \xi_j \]

should hold.
The goal is to design an objective function that minimizes $\epsilon$ and $\xi$ and maximizes $\delta$. The optimization problem should also solve for $w$ and $b$, and for this some constraint has to be placed on $w$. Another goal is to try to use the dual program to solve the optimization problem, because the solutions involve inner products, and thus the problem is amenable to a generalization using kernel functions.

The first attempt, which is to use the objective function

$$J(w, \epsilon, \xi, b, \delta) = -\delta + K(\epsilon^\top \xi^\top)1_{p+q}$$

and the constraint $w^\top w \leq 1$ does not work very well, because this constraint needs to be guarded by a Lagrange multiplier $\gamma \geq 0$, and as a result, minimizing the Lagrangian $L$ to find the dual function $G$ gives an equation for solving $w$ of the form

$$2\gamma w = -X^\top (\lambda)$$

but if the sets $\{u_i\}_{i=1}^p$ and $\{v_j\}_{j=1}^q$ are not linearly separable, then an optimal solution may occur for $\gamma = 0$, in which case it is impossible to determine $w$. This is Problem (SVM$_{s1}$) considered in Section 34.1.

**Soft margin SVM (SVM$_{s1}$):**

$$\text{minimize} \quad -\delta + K\left(\sum_{i=1}^p \epsilon_i + \sum_{j=1}^q \xi_j\right)$$

subject to

$$w^\top u_i - b \geq \delta - \epsilon_i, \quad \epsilon_i \geq 0 \quad i = 1, \ldots, p$$
$$-w^\top v_j + b \geq \delta - \xi_j, \quad \xi_j \geq 0 \quad j = 1, \ldots, q$$
$$w^\top w \leq 1.$$ 

It is customary to write $\ell = p + q$.

It is shown in Section 34.1 that the dual program is equivalent to the following minimization program:

$$\text{minimize} \quad (\lambda^\top \mu^\top) X^\top X \begin{pmatrix} \lambda \\ \mu \end{pmatrix}$$

subject to

$$\sum_{i=1}^p \lambda_i = \sum_{j=1}^q \mu_j = \frac{1}{2}$$
$$0 \leq \lambda_i \leq K, \quad i = 1, \ldots, p$$
$$0 \leq \mu_j \leq K, \quad j = 1, \ldots, q.$$
Observe that the constraints imply that $K$ must be chosen so that

\[ K \geq \max \left\{ \frac{1}{2p}, \frac{1}{2q} \right\}. \]

If the optimal value is 0, then $\gamma = 0$ and $X \begin{pmatrix} \lambda \\ \mu \end{pmatrix} = 0$, so in this case it is not possible to determine $w$. However, if the optimal value is $> 0$, then once a solution for $\lambda$ and $\mu$ is obtained, we have

\[ \gamma = \frac{1}{2} \left( (\lambda^\top \mu^\top) X^\top X \begin{pmatrix} \lambda \\ \mu \end{pmatrix} \right)^{1/2} \]

\[ w = \frac{1}{2\gamma} \left( \sum_{i=1}^{p} \lambda_i u_i - \sum_{j=1}^{q} \mu_j v_j \right), \]

so we get

\[ w = \frac{\sum_{i=1}^{p} \lambda_i u_i - \sum_{j=1}^{q} \mu_j v_j}{\left( (\lambda^\top \mu^\top) X^\top X \begin{pmatrix} \lambda \\ \mu \end{pmatrix} \right)^{1/2}}, \]

If the following mild hypothesis holds then $b$ and $\delta$ can be found.

**Standard Margin Hypothesis** for (SVM$_{s1}$). There is some index $i_0$ such that $0 < \lambda_{i_0} < K$ and there is some index $j_0$ such that $0 < \mu_{j_0} < K$. This means that some $u_{i_0}$ is correctly classified and on the blue margin, and some $v_{j_0}$ is correctly classified and on the red margin.

If the **Standard Margin Hypothesis** for (SVM$_{s1}$) holds then $\epsilon_{i_0} = 0$ and $\mu_{j_0} = 0$, and then we have the active equations

\[ w^\top u_{i_0} - b = \delta \quad \text{and} \quad -w^\top v_{j_0} + b = \delta, \]

and we obtain the value of $b$ and $\delta$ as

\[ b = \frac{1}{2} (w^\top u_{i_0} + w^\top v_{j_0}) \]

\[ \delta = \frac{1}{2} (w^\top u_{i_0} - w^\top v_{j_0}). \]

The second more successful approach is to add the term $(1/2)w^\top w$ to the objective function and to drop the constraint $w^\top w \leq 1$. Then there are several variants of this method, depending on the choice of the regularizing term involving $\epsilon$ and $\xi$ (linear or quadratic), how
the margin is dealt with (implicitly with the term 1 or explicit with a term \( \eta \)), and whether the term \( (1/2)b^2 \) is added to the objective function or not.

These methods all share the property that if the primal problem has an optimal solution with \( w \neq 0 \), then the dual problem always determines \( w \), and then under mild conditions that we call standard margin hypotheses, \( b \) and \( \eta \) can be determined. Then \( \epsilon \) and \( \xi \) can be determined using the constraints that are active. When \( (1/2)b^2 \) is added to the objective function, \( b \) is determined by the equation

\[
b = -(1_p^T \lambda - 1_q^T \mu).
\]

All these problems are convex and the constraints are qualified, so the duality gap is zero, and if the primal has an optimal solution with \( w \neq 0 \), then it follows that \( \eta \geq 0 \).

We now consider five variants in more details.

(1) Basic soft margin SVM: (SVM\(_{s2}\)).

This is the optimization problem in which the regularization term \( K(\epsilon^T \xi^T)1_{p+q} \) is linear and the margin \( \delta \) is given by \( \delta = 1/\|w\| \):

\[
\text{minimize } \frac{1}{2} w^T w + K(\epsilon^T \xi^T) 1_{p+q} \\
\text{subject to } \\
w^T u_i - b \geq 1 - \epsilon_i, \quad \epsilon_i \geq 0 \quad i = 1, \ldots, p \\
-w^T v_j + b \geq 1 - \xi_j, \quad \xi_j \geq 0 \quad j = 1, \ldots, q.
\]

This problem is the classical one discussed in all books on machine learning or pattern analysis, for instance Vapnik [111], Bishop [18], and Shawe–Taylor and Christianini [97]. It is shown in Section 34.2 that the dual program is

\[
\text{minimize } \frac{1}{2} (\lambda^T \mu^T) X^T X \left(\begin{array}{c}
\lambda \\
\mu
\end{array}\right) - (\lambda^T \mu^T) 1_{p+q} \\
\text{subject to } \\
\sum_{i=1}^{p} \lambda_i = \sum_{j=1}^{q} \mu_j \\
0 \leq \lambda_i \leq K, \quad i = 1, \ldots, p \\
0 \leq \mu_j \leq K, \quad j = 1, \ldots, q.
\]

We can use the dual program to solve the primal. Once \( \lambda \geq 0, \mu \geq 0 \) have been found, \( w \) is given by

\[
w = -X \left(\begin{array}{c}
\lambda \\
\mu
\end{array}\right) = \sum_{i=1}^{p} \lambda_i u_i - \sum_{j=1}^{q} \mu_j v_j,
\]
but $b$ is not determined by the dual.

The complementary slackness conditions imply that if $\epsilon_i > 0$ then $\lambda_i = K$, and if $\xi_j > 0$, then $\mu_j = K$. Consequently, if $\lambda_i < K$ then $\epsilon_i = 0$ and $u_i$ is correctly classified, and similarly if $\mu_j < K$ then $\xi_j = 0$ and $v_j$ is correctly classified.

A priori nothing prevents the situation where $\lambda_i = K$ for all nonzero $\lambda_i$ or $\mu_j = K$ for all nonzero $\mu_j$. If this happens, we can rerun the optimization method with a larger value of $K$. If the following mild hypothesis holds then $b$ can be found.

**Standard Margin Hypothesis** for (SVM$_s^2$). There is some index $i_0$ such that $0 < \lambda_{i_0} < K$ and there is some index $j_0$ such that $0 < \mu_{j_0} < K$. This means that some $u_{i_0}$ is correctly classified and on the blue margin, and some $v_{j_0}$ is correctly classified and on the red margin.

If the **Standard Margin Hypothesis** for (SVM$_s^2$) holds then $\epsilon_{i_0} = 0$ and $\mu_{j_0} = 0$, and then we have the active equations

$$w^\top u_{i_0} - b = 1 \quad \text{and} \quad -w^\top v_{j_0} + b = 1,$$

and we obtain

$$b = \frac{1}{2}(w^\top u_{i_0} + w^\top v_{j_0}).$$

(2) **Basic Soft margin $\nu$-SVM Problem** (SVM$_{s^2}$).

This a generalization of Problem (SVM$_{s^2}$) for a version of the soft margin SVM coming from Problem (SVM$_{h^2}$), obtained by adding an extra degree of freedom, namely instead of the margin $\delta = 1/\|w\|$, we use the margin $\delta = \eta/\|w\|$ where $\eta$ is some positive constant that we wish to maximize. To do so, we add a term $-K_m\eta$ to the objective function. We have the following optimization problem:

$$\begin{align*}
\text{minimize} & \quad \frac{1}{2}w^\top w - K_m\eta + K_s \left( \epsilon^\top \xi^\top \right) 1_{p+q} \\
\text{subject to} & \quad w^\top u_i - b \geq \eta - \epsilon_i, \quad \epsilon_i \geq 0 \quad i = 1, \ldots, p \\
& \quad -w^\top v_j + b \geq \eta - \xi_j, \quad \xi_j \geq 0 \quad j = 1, \ldots, q \\
& \quad \eta \geq 0,
\end{align*}$$

where $K_m > 0$ and $K_s > 0$ are fixed constants that can be adjusted to determine the influence of $\eta$ and the regularizing term.

This version of the SVM problem was first discussed in Schölkopf, Smola, Williamson, and Bartlett [88] under the name of $\nu$-SVC, and also used in Schölkopf, Platt, Shawe-Taylor, and Smola [87].
In order for the problem to have a solution we must pick $K_m$ and $K_s$ so that
\[ K_m \leq \min\{2pK_s, 2qK_s\}. \]

It is shown in Section 34.3 that the dual program is
\[
\begin{align*}
\text{minimize} \quad & \frac{1}{2} (\lambda^T \mu^T) X^T X \begin{pmatrix} \lambda \\ \mu \end{pmatrix} \\
\text{subject to} \quad & \sum_{i=1}^{p} \lambda_i = \sum_{j=1}^{q} \mu_j \\
& \sum_{i=1}^{p} \lambda_i + \sum_{j=1}^{q} \mu_j \geq K_m \\
& 0 \leq \lambda_i \leq K_s, \quad i = 1, \ldots, p \\
& 0 \leq \mu_j \leq K_s, \quad j = 1, \ldots, q.
\end{align*}
\]

If the primal problem has an optimal solution with $w \neq 0$, then using the fact that the duality gap is zero we can show that $\eta \geq 0$. Thus constraint $\eta \geq 0$ could be omitted. As in the previous case $w$ is given by
\[ w = -X \begin{pmatrix} \lambda \\ \mu \end{pmatrix} = \sum_{i=1}^{p} \lambda_i u_i - \sum_{j=1}^{q} \mu_j v_j, \]

but $b$ and $\eta$ are not determined by the dual.

If we drop the constraint $\eta \geq 0$, then the inequality
\[ \sum_{i=1}^{p} \lambda_i + \sum_{j=1}^{q} \mu_j \geq K_m \]
is replaced by the equation
\[ \sum_{i=1}^{p} \lambda_i + \sum_{j=1}^{q} \mu_j = K_m. \]

It convenient to define $\nu > 0$ such that
\[ K_m = (p + q)K_s \nu, \]

that is
\[ \nu = \frac{K_m}{(p + q)K_s}, \]
so that the objective function $J(w, \epsilon, \xi, b, \eta)$ is given by

$$J(w, \epsilon, \xi, b, \eta) = \frac{1}{2} w^\top w + K \left( -\nu \eta + \frac{1}{p+q} \left( \epsilon^\top \xi^\top \right) 1_{p+q} \right),$$

with $K = (p+q)K_s$, and so $K_m = K\nu$ and $K_s = K/(p+q)$.

Observe that the condition $K_m \leq \min\{2pK_s, 2qK_s\}$ is equivalent to

$$\nu \leq \min\left\{ \frac{2p}{p+q}, \frac{2q}{p+q} \right\} \leq 1.$$ 

Since we obtain an equivalent problem by rescaling by a common positive factor, it is convenient to normalize $K_s$ as

$$K_s = \frac{1}{p+q},$$

in which case $K_m = \nu$. This method is called the $\nu$-support vector machine.

Under the **Standard Margin Hypothesis** for (SVMs), there is some $i_0$ such that $0 < \lambda_{i_0} < K_s$ and some $j_0$ such that $0 < \mu_{j_0} < K_s$, and by the complementary slackness conditions $\epsilon_{i_0} = 0$ and $\xi_{j_0} = 0$, so we have the two active constraints

$$w^\top u_{i_0} - b = \eta, \quad -w^\top v_{j_0} + b = \eta,$$

and we can solve for $b$ and $\eta$ and we get

$$b = \frac{w^\top u_{i_0} + w^\top v_{j_0}}{2} \quad \eta = \frac{w^\top u_{i_0} - w^\top v_{j_0}}{2}.$$

Proposition 34.1 gives an upper bound on the number of points $u_i$ and the number of points $v_j$ that fail to achieve the margin, and that have margin at most $\eta$. As a consequence, if the $u_i$s and $v_j$s are not linearly separable we must pick $\nu$ such that $2/(p+q) \leq \nu \leq \min\{2p/(p+q), 2q/(p+q)\}$ for the method to succeed.

We also investigate conditions on $\nu$ that ensure that either some point $u_i$ is correctly classified or some point $v_i$ is correctly classified, and the corresponding constraint is active (so that $u_i$ is on the margin, resp. $v_j$ is on the margin). If there are $p_f$ misclassified points $u_i$ and $q_f$ misclassified points $v_j$, then if $p_f + q_f \geq 3$ and $2/(p+q) < (p_f + q_f)/(p+q)$, then the above property holds; see Proposition 34.2. We also show that if $p_f, q_f \geq 2$ and if $2/(p+q) < 4/(p+q)$, then $b$ and $\eta$ can be found without reference to the standard margin hypothesis; see Proposition 34.3.

(3) **Basic Quadratic Soft margin $\nu$-SVM Problem (SVMs).** This is the version of Problem (SVMs) in which instead of using the linear function $K_s \left( \epsilon^\top \xi^\top \right) 1_{p+q}$ as a regularizing
function we use the quadratic function $K(\|\epsilon\|_2^2 + \|\xi\|_2^2)$. The optimization problem is

$$\begin{align*}
&\text{minimize} \quad \frac{1}{2}w^\top w - \nu \eta + K(\epsilon^\top \epsilon + \xi^\top \xi) \\
&\text{subject to} \\
&\quad w^\top u_i - b \geq \eta - \epsilon_i, \quad i = 1, \ldots, p \\
&\quad -w^\top v_j + b \geq \eta - \xi_j, \quad j = 1, \ldots, q \\
&\quad \eta \geq 0,
\end{align*}$$

where $\nu$ and $K$ are two given positive constants. As we saw earlier, it is convenient to pick $K = 1/(p + q)$.

In this method, it is no longer necessary to require $\epsilon \geq 0$ and $\xi \geq 0$, because an optimal solution satisfies these conditions. We can also omit the constraint $\eta \geq 0$, because for an optimal solution it can be shown using duality that $\eta \geq 0$. It is shown in Section 34.4 that the dual is given by

$$\begin{align*}
&\text{minimize} \quad \frac{1}{2} \begin{pmatrix} \lambda^\top & \mu^\top \end{pmatrix} \left( X^\top X + \frac{1}{2K}I_{p+q} \right) \begin{pmatrix} \lambda \\ \mu \end{pmatrix} \\
&\text{subject to} \\
&\quad \sum_{i=1}^{p} \lambda_i = \sum_{j=1}^{q} \mu_j \\
&\quad \sum_{i=1}^{p} \lambda_i + \sum_{j=1}^{q} \mu_j \geq \nu \\
&\quad \lambda_i \geq 0, \quad i = 1, \ldots, p \\
&\quad \mu_j \geq 0, \quad j = 1, \ldots, q.
\end{align*}$$

The above program is similar to the program that was obtained for Problem (SVM$_{s2'}$) but the matrix $X^\top X$ is replaced by the matrix $X^\top X + (1/2K)I_{p+q}$, which is positive definite since $K > 0$, and also the inequalities $\lambda_i \leq K$ and $\mu_j \leq K$ no longer hold. However, the constraints imply that there is some $i_0$ such that $\lambda_{i_0} > 0$ and some $j_0$ such that $\mu_{j_0} > 0$. If the constraint $\eta \geq 0$ is dropped, then the inequality

$$\sum_{i=1}^{p} \lambda_i + \sum_{j=1}^{q} \mu_j \geq \nu$$

is replaced by the equation

$$\sum_{i=1}^{p} \lambda_i + \sum_{j=1}^{q} \mu_j = \nu.$$
We obtain \( w \) from \( \lambda \) and \( \mu \), and \( \gamma \), as in Problem (SVM_{s2'}); namely,

\[
w = -X \begin{pmatrix} \lambda \\ \mu \end{pmatrix} = \sum_{i=1}^{p} \lambda_i u_i - \sum_{j=1}^{q} \mu_j v_j,
\]

but the dual does not determine \( b \) and \( \eta \). However, \( \epsilon \) and \( \xi \) are determined by

\[
\epsilon = \frac{{\lambda}}{2K}, \quad \xi = \frac{{\mu}}{2K}.
\]

Also since the constraints

\[
\sum_{i=1}^{p} \lambda_i \geq \frac{\nu}{2} \quad \text{and} \quad \sum_{j=1}^{q} \mu_j \geq \frac{\nu}{2}
\]

imply that there is some \( i_0 \) such that \( \lambda_{i_0} > 0 \) and some \( j_0 \) such that \( \mu_{j_0} > 0 \), we have \( \epsilon_{i_0} > 0 \) and \( \xi_{j_0} > 0 \), which means that at least two points are misclassified, so Problem (SVM_{s3}) should only be used when the sets \( \{u_i\} \) and \( \{v_j\} \) are not linearly separable. We can solve for \( b \) and \( \eta \) using the active constraints corresponding to any \( i_0 \) such that \( \lambda_{i_0} > 0 \) and any \( j_0 \) such that \( \mu_{j_0} > 0 \). With this method, there is no need for a standard margin hypothesis.

(4) **Soft margin \( \nu \)-SVM Problem (SVM_{s4})**. This is the variation of Problem (SVM_{s2'}) obtained by adding the term \((1/2)b^2\) to the objective function. The result is that in minimizing the Lagrangian to find the dual function \( G \), not just \( w \) but also \( b \) is determined. We also suppress the constraint \( \eta \geq 0 \) which turns out to be redundant. The optimization problem is

\[
\begin{align*}
& \text{minimize} \quad \frac{1}{2} w^\top w + \frac{1}{2} b^2 - \nu \eta + K_s (\epsilon^\top \xi^\top) 1_{p+q} \\
& \text{subject to} \quad
\begin{align*}
& w^\top u_i - b \geq \eta - \epsilon_i, \quad \epsilon_i \geq 0 \quad i = 1, \ldots, p \\
& -w^\top v_j + b \geq \eta - \xi_j, \quad \xi_j \geq 0 \quad j = 1, \ldots, q,
\end{align*}
\end{align*}
\]

with \( K_s = 1/(p+q) \).

It is shown in Section 34.5 that the dual is given by

\[
\begin{align*}
& \text{minimize} \quad \frac{1}{2} \begin{pmatrix} \lambda^\top \\ \mu^\top \end{pmatrix} \left( X^\top X + \begin{pmatrix} 1_p 1_p^\top \\ -1_q 1_p^\top & -1_p 1_q^\top \end{pmatrix} \right) \begin{pmatrix} \lambda \\ \mu \end{pmatrix} \\
& \text{subject to} \quad
\begin{align*}
& \sum_{i=1}^{p} \lambda_i + \sum_{j=1}^{q} \mu_j = \nu \\
& 0 \leq \lambda_i \leq K_s, \quad i = 1, \ldots, p \\
& 0 \leq \mu_j \leq K_s, \quad j = 1, \ldots, q.
\end{align*}
\end{align*}
\]
Once a solution for $\lambda$ and $\mu$ is obtained, we have

$$w = -X \begin{pmatrix} \lambda \\ \mu \end{pmatrix} = \sum_{i=1}^{p} \lambda_i u_i - \sum_{j=1}^{q} \mu_j v_j$$

$$b = -\sum_{i=1}^{p} \lambda_i + \sum_{j=1}^{q} \mu_j,$$

but $\eta$ is not determined by the dual. Note that the constraint

$$\sum_{i=1}^{p} \lambda_i = \sum_{j=1}^{q} \mu_j$$

occurring in the dual of Program (SVM\textsubscript{s2'}) has been traded for the equation

$$b = -\sum_{i=1}^{p} \lambda_i + \sum_{j=1}^{q} \mu_j$$

determining $b$. This seems to be an advantage of Problem (SVM\textsubscript{s4}).

It is also shown that if the primal problem (SVM\textsubscript{s4}) has an optimal solution with $w \neq 0$, then $\eta \geq 0$. In order for the primal to have a solution we must have $\nu \leq 1$.

Under the **Standard Margin Hypothesis** for (SVM\textsubscript{s4}), either there is some $i_0$ such that $0 < \lambda_{i_0} < K_s$ or there is some $j_0$ such that $0 < \mu_{j_0} < K_s$, and by the complementary slackness conditions $\epsilon_{i_0} = 0$ or $\xi_{j_0} = 0$, so we have

$$w^\top u_{i_0} - b = \eta, \quad \text{or} \quad -w^\top v_{j_0} + b = \eta,$$

and we can solve for $\eta$.

Proposition 34.4 gives an upper bound on the number of points $u_i$ and the number of points $v_j$ that fail to achieve the margin, and that have margin at most $\eta$. As a consequence, if the $u_i$s and $v_j$s are not linearly separable we must pick $\nu$ such that $1/(p+q) \leq \nu \leq 1$ for the method to succeed.

We also investigate conditions on $\nu$ that ensure that either some point $u_i$ is correctly classified or some point $v_i$ is correctly classified, and the corresponding constraint is active (so that $u_i$ is on the margin, resp. $v_i$ is on the margin). If there are $p_f$ misclassified points $u_i$ and $q_f$ misclassified points $v_j$, then if $p_f + q_f \geq 2$ and $1/(p+q) < (p_f + q_f)/(p + q)$, then the above property holds. See Proposition 34.5; this is a slight improvement over Proposition 34.2. We also show that if $p_f + q_f \geq 2$ and if $1/(p+q) < 3/(p+q)$, then $\eta$ can be found without requiring the standard margin hypothesis; see Proposition 34.6. This is also a slight improvement over Proposition 34.3.
Quadratic Soft margin $\nu$-SVM Problem ($\text{SVM}_{s3}$). This is the variant of Problem ($\text{SVM}_{s3}$) in which we add the term $(1/2)b^2$ to the objective function. We also drop the constraint $\eta \geq 0$ which is redundant. We have the following optimization problem:

$$
\text{minimize} \quad \frac{1}{2} w^\top w + \frac{1}{2} b^2 - \nu \eta + K(\epsilon^\top \epsilon + \xi^\top \xi)
$$

subject to

$$
w^\top u_i - b \geq \eta - \epsilon_i, \quad i = 1, \ldots, p$$

$$-w^\top v_j + b \geq \eta - \xi_j, \quad j = 1, \ldots, q,$$

where $\nu$ and $K$ are two given positive constants. As we saw earlier, it is convenient to pick $K = 1/(p + q)$.

It is shown in Section 34.6 that the dual of Program ($\text{SVM}_{s3}$) is given by

$$
\text{minimize} \quad \frac{1}{2} (\lambda^\top \mu^\top) \left( X^\top X + \begin{pmatrix} 1_p & 1_p^\top \\ -1_q & 1_q^\top \end{pmatrix} + \frac{1}{2K} I_{p+q} \right) \begin{pmatrix} \lambda \\ \mu \end{pmatrix}
$$

subject to

$$
\sum_{i=1}^p \lambda_i + \sum_{j=1}^q \mu_j = \nu
$$

$$\lambda_i \geq 0, \quad i = 1, \ldots, p$$

$$\mu_j \geq 0, \quad j = 1, \ldots, q.$$

This time we obtain $w$, $b$, $\epsilon$ and $\xi$ from $\lambda$ and $\mu$:

$$w = \sum_{i=1}^p \lambda_i u_i - \sum_{j=1}^q \mu_j v_j$$

$$b = - \sum_{i=1}^p \lambda_i + \sum_{j=1}^q \mu_j$$

$$\epsilon = \frac{\lambda}{2K}$$

$$\xi = \frac{\mu}{2K}.$$

The constraint

$$\sum_{i=1}^p \lambda_i = \sum_{j=1}^q \mu_j$$

occurring in the dual of Program ($\text{SVM}_{s3}$) has been traded for the equation

$$b = - \sum_{i=1}^p \lambda_i + \sum_{j=1}^q \mu_j$$
determining $b$. This seems to be an advantage of Problem (SVM$_{s5}$).

The constraint

$$\sum_{i=1}^{p} \lambda_i + \sum_{j=1}^{q} \mu_j = \nu$$

implies that either there is some $i_0$ such that $\lambda_{i_0} > 0$ or there is some $j_0$ such that $\mu_{j_0} > 0$, we have $\epsilon_{i_0} > 0$ or $\xi_{j_0} > 0$, which means that at least one point is misclassified, so Problem (SVM$_{s5}$) should only be used when the sets $\{u_i\}$ and $\{v_j\}$ are not linearly separable. We can solve for $\eta$ using the active constraints corresponding to any $i_0$ such that $\lambda_{i_0} > 0$ or any $j_0$ such that $\mu_{j_0} > 0$. Using duality, it can be shown that if the primal has an optimal solution with $w \neq 0$, then $\eta \geq 0$.

These methods all have a kernelized version.

In summary, from a theoretical point of view, Problems (SVM$_{s4}$) and (SVM$_{s5}$) seem to have more advantages than the others since they determine at least $w$ and $b$, but this remains to be verified experimentally.
Part V
Appendix
Appendix A

Total Orthogonal Families in Hilbert Spaces

A.1 Total Orthogonal Families (Hilbert Bases), Fourier Coefficients

We conclude our quick tour of Hilbert spaces by showing that the notion of orthogonal basis can be generalized to Hilbert spaces. However, the useful notion is not the usual notion of a basis, but a notion which is an abstraction of the concept of Fourier series. Every element of a Hilbert space is the “sum” of its Fourier series.

Definition A.1. Given a Hilbert space $E$, a family $(u_k)_{k \in K}$ of nonnull vectors is an orthogonal family iff the $u_k$ are pairwise orthogonal, i.e., $\langle u_i, u_j \rangle = 0$ for all $i \neq j$ ($i, j \in K$), and an orthonormal family iff $\langle u_i, u_j \rangle = \delta_{i,j}$, for all $i, j \in K$. A total orthogonal family (or system) or Hilbert basis is an orthogonal family that is dense in $E$. This means that for every $v \in E$, for every $\epsilon > 0$, there is some finite subset $I \subseteq K$ and some family $(\lambda_i)_{i \in I}$ of complex numbers, such that

$$\left\| v - \sum_{i \in I} \lambda_i u_i \right\| < \epsilon.$$

Given an orthogonal family $(u_k)_{k \in K}$, for every $v \in E$, for every $k \in K$, the scalar $c_k = \langle v, u_k \rangle / \|u_k\|^2$ is called the $k$-th Fourier coefficient of $v$ over $(u_k)_{k \in K}$.

Remark: The terminology Hilbert basis is misleading, because a Hilbert basis $(u_k)_{k \in K}$ is not necessarily a basis in the algebraic sense. Indeed, in general, $(u_k)_{k \in K}$ does not span $E$. Intuitively, it takes linear combinations of the $u_k$’s with infinitely many nonnull coefficients to span $E$. Technically, this is achieved in terms of limits. In order to avoid the confusion between bases in the algebraic sense and Hilbert bases, some authors refer to algebraic bases as Hamel bases and to total orthogonal families (or Hilbert bases) as Schauder bases.
Appendix A. Total Orthogonal Families in Hilbert Spaces

Given an orthogonal family \((u_k)_{k \in K}\), for any finite subset \(I\) of \(K\), we often call sums of the form \(\sum_{i \in I} \lambda_i u_i\) partial sums of Fourier series, and if these partial sums converge to a limit denoted as \(\sum_{k \in K} c_k u_k\), we call \(\sum_{k \in K} c_k u_k\) a Fourier series.

However, we have to make sense of such sums! Indeed, when \(K\) is unordered or uncountable, the notion of limit or sum has not been defined. This can be done as follows (for more details, see Dixmier [35]):

**Definition A.2.** Given a normed vector space \(E\) (say, a Hilbert space), for any nonempty index set \(K\), we say that a family \((u_k)_{k \in K}\) of vectors in \(E\) is summable with sum \(v \in E\) iff for every \(\epsilon > 0\), there is some finite subset \(I\) of \(K\), such that,

\[
\left\| v - \sum_{j \in J} u_j \right\| < \epsilon
\]

for every finite subset \(J\) with \(I \subseteq J \subseteq K\). We say that the family \((u_k)_{k \in K}\) is summable iff there is some \(v \in E\) such that \((u_k)_{k \in K}\) is summable with sum \(v\). A family \((u_k)_{k \in K}\) is a Cauchy family iff for every \(\epsilon > 0\), there is a finite subset \(I\) of \(K\), such that,

\[
\left\| \sum_{j \in J} u_j \right\| < \epsilon
\]

for every finite subset \(J\) of \(K\) with \(I \cap J = \emptyset\).

If \((u_k)_{k \in K}\) is summable with sum \(v\), we usually denote \(v\) as \(\sum_{k \in K} u_k\). The following technical proposition will be needed:

**Proposition A.1.** Let \(E\) be a complete normed vector space (say, a Hilbert space).

1. For any nonempty index set \(K\), a family \((u_k)_{k \in K}\) is summable iff it is a Cauchy family.

2. Given a family \((r_k)_{k \in K}\) of nonnegative reals \(r_k \geq 0\) such that \(\sum_{i \in I} r_i < B\) for every finite subset \(I\) of \(K\), then \((r_k)_{k \in K}\) is summable and \(\sum_{k \in K} r_k = r\), where \(r\) is least upper bound of the set of finite sums \(\sum_{i \in I} r_i\) \((I \subseteq K)\).

**Proof.** (1) If \((u_k)_{k \in K}\) is summable, for every finite subset \(I\) of \(K\), let

\[ u_I = \sum_{i \in I} u_i \quad \text{and} \quad u = \sum_{k \in K} u_k \]

For every \(\epsilon > 0\), there is some finite subset \(I\) of \(K\) such that

\[ \|u - u_I\| < \epsilon/2 \]

for all finite subsets \(L\) such that \(I \subseteq L \subseteq K\). For every finite subset \(J\) of \(K\) such that \(I \cap J = \emptyset\), since \(I \subseteq I \cup J \subseteq K\) and \(I \cup J\) is finite, we have

\[ \|u - u_{I \cup J}\| < \epsilon/2 \quad \text{and} \quad \|u - u_I\| < \epsilon/2, \]

\[
\|v - \sum_{j \in J} u_j\| < \epsilon
\]

for every finite subset \(J\) with \(I \subseteq J \subseteq K\). We say that the family \((u_k)_{k \in K}\) is summable iff there is some \(v \in E\) such that \((u_k)_{k \in K}\) is summable with sum \(v\). A family \((u_k)_{k \in K}\) is a Cauchy family iff for every \(\epsilon > 0\), there is a finite subset \(I\) of \(K\), such that,

\[
\left\| \sum_{j \in J} u_j \right\| < \epsilon
\]

for every finite subset \(J\) of \(K\) with \(I \cap J = \emptyset\),
and since
\[ \|u_{I \cup J} - u_I\| \leq \|u_{I \cup J} - u\| + \|u - u_I\| \]
and \( u_{I \cup J} - u_I = u_J \) since \( I \cap J = \emptyset \), we get
\[ \|u_J\| = \|u_{I \cup J} - u_I\| < \epsilon, \]
which is the condition for \((u_k)_{k \in K}\) to be a Cauchy family.

Conversely, assume that \((u_k)_{k \in K}\) is a Cauchy family. We define inductively a decreasing sequence \((X_n)\) of subsets of \(E\), each of diameter at most \(1/n\), as follows: For \(n = 1\), since \((u_k)_{k \in K}\) is a Cauchy family, there is some finite subset \(J_1\) of \(K\) such that
\[ \|u_{J_1}\| < 1/2 \]
for every finite subset \(J\) of \(K\) with \(J_1 \cap J = \emptyset\). We pick some finite subset \(J_1\) with the above property, and we let \(I_1 = J_1\) and
\[ X_1 = \{u_I \mid I_1 \subseteq I \subseteq K, I \text{ finite}\}. \]

For \(n \geq 1\), there is some finite subset \(J_{n+1}\) of \(K\) such that
\[ \|u_{J_{n+1}}\| < 1/(2n + 2) \]
for every finite subset \(J\) of \(K\) with \(J_{n+1} \cap J = \emptyset\). We pick some finite subset \(J_{n+1}\) with the above property, and we let \(I_{n+1} = I_n \cup J_{n+1}\) and
\[ X_{n+1} = \{u_I \mid I_{n+1} \subseteq I \subseteq K, I \text{ finite}\}. \]

Since \(I_n \subseteq I_{n+1}\), it is obvious that \(X_{n+1} \subseteq X_n\) for all \(n \geq 1\). We need to prove that each \(X_n\) has diameter at most \(1/n\). Since \(J_n\) was chosen such that
\[ \|u_{J_n}\| < 1/(2n) \]
for every finite subset \(J\) of \(K\) with \(J_n \cap J = \emptyset\), and since \(J_n \subseteq I_n\), it is also true that
\[ \|u_{J_n}\| < 1/(2n) \]
for every finite subset \(J\) of \(K\) with \(I_n \cap J = \emptyset\). Then, for every two finite subsets \(J, L\) such that \(I_n \subseteq J, L \subseteq K\), we have
\[ \|u_{J - I_n}\| < 1/(2n) \quad \text{and} \quad \|u_{L - I_n}\| < 1/(2n), \]
and since
\[ \|u_J - u_L\| \leq \|u_J - u_{I_n}\| + \|u_{I_n} - u_L\| = \|u_{J - I_n}\| + \|u_{L - I_n}\|, \]
we get
\[ \|u_J - u_L\| < 1/n, \]
which proves that $\delta(X_n) \leq 1/n$. Now, if we consider the sequence of closed sets $(X_n)$, we still have $X_{n+1} \subseteq X_n$, and by Proposition 29.4, $\delta(X_n) = \delta(X_n) \leq 1/n$, which means that $\lim_{n \to \infty} \delta(X_n) = 0$, and by Proposition 29.4, $\bigcap_{n=1}^{\infty} X_n$ consists of a single element $u$. We claim that $u$ is the sum of the family $(u_k)_{k \in K}$.

For every $\epsilon > 0$, there is some $n \geq 1$ such that $n > 2/\epsilon$, and since $u \in \overline{X_m}$ for all $m \geq 1$, there is some finite subset $J_0$ of $K$ such that $I_n \subseteq J_0$ and

$$\|u - u_{J_0}\| < \epsilon/2,$$

where $I_n$ is the finite subset of $K$ involved in the definition of $X_n$. However, since $\delta(X_n) \leq 1/n$, for every finite subset $J$ of $K$ such that $I_n \subseteq J$, we have

$$\|u_J - u_{J_0}\| \leq 1/n < \epsilon/2,$$

and since

$$\|u - u_J\| \leq \|u - u_{J_0}\| + \|u_{J_0} - u_J\|,$$

we get

$$\|u - u_J\| < \epsilon$$

for every finite subset $J$ of $K$ with $I_n \subseteq J$, which proves that $u$ is the sum of the family $(u_k)_{k \in K}$.

(2) Since every finite sum $\sum_{i \in I} r_i$ is bounded by the uniform bound $B$, the set of these finite sums has a least upper bound $r \leq B$. For every $\epsilon > 0$, since $r$ is the least upper bound of the finite sums $\sum_{i \in I} r_i$ (where $I$ finite, $I \subseteq K$), there is some finite $I \subseteq K$ such that

$$\left| r - \sum_{i \in I} r_i \right| < \epsilon,$$

and since $r_k \geq 0$ for all $k \in K$, we have

$$\sum_{i \in I} r_i \leq \sum_{j \in J} r_j$$

whenever $I \subseteq J$, which shows that

$$\left| r - \sum_{j \in J} r_j \right| \leq \left| r - \sum_{i \in I} r_i \right| < \epsilon$$

for every finite subset $J$ such that $I \subseteq J \subseteq K$, proving that $(r_k)_{k \in K}$ is summable with sum

$$\sum_{k \in K} r_k = r.$$
Remark: The notion of summability implies that the sum of a family \((u_k)_{k \in K}\) is independent of any order on \(K\). In this sense, it is a kind of “commutative summability”. More precisely, it is easy to show that for every bijection \(\varphi: K \rightarrow K\) (intuitively, a reordering of \(K\)), the family \((u_k)_{k \in K}\) is summable iff the family \((u_l)_{l \in \varphi(K)}\) is summable, and if so, they have the same sum.

The following proposition gives some of the main properties of Fourier coefficients. Among other things, at most countably many of the Fourier coefficient may be nonnull, and the partial sums of a Fourier series converge. Given an orthogonal family \((u_k)_{k \in K}\), we let \(U_k = \mathbb{C}u_k\), and \(p_{U_k}: E \rightarrow U_k\) is the projection of \(E\) onto \(U_k\).

Proposition A.2. Let \(E\) be a Hilbert space, \((u_k)_{k \in K}\) an orthogonal family in \(E\), and \(V\) the closure of the subspace generated by \((u_k)_{k \in K}\). The following properties hold:

1. For every \(v \in E\), for every finite subset \(I \subseteq K\), we have
   \[
   \sum_{i \in I} |c_i|^2 \leq \|v\|^2,
   \]
   where the \(c_k\) are the Fourier coefficients of \(v\).

2. For every vector \(v \in E\), if \((c_k)_{k \in K}\) are the Fourier coefficients of \(v\), the following conditions are equivalent:
   
   (2a) \(v \in V\)
   
   (2b) The family \((c_ku_k)_{k \in K}\) is summable and \(v = \sum_{k \in K} c_ku_k\).
   
   (2c) The family \((|c_k|^2)_{k \in K}\) is summable and \(\|v\|^2 = \sum_{k \in K} |c_k|^2\);

3. The family \((|c_k|^2)_{k \in K}\) is summable, and we have the Bessel inequality:
   \[
   \sum_{k \in K} |c_k|^2 \leq \|v\|^2.
   \]

As a consequence, at most countably many of the \(c_k\) may be nonzero. The family \((c_ku_k)_{k \in K}\) forms a Cauchy family, and thus, the Fourier series \(\sum_{k \in K} c_ku_k\) converges in \(E\) to some vector \(u = \sum_{k \in K} c_ku_k\). Furthermore, \(u = p_V(v)\).

Proof. (1) Let
   \[
   u_I = \sum_{i \in I} c_iu_i
   \]
for any finite subset \(I\) of \(K\). We claim that \(v - u_I\) is orthogonal to \(u_i\) for every \(i \in I\). Indeed,

\[
\langle v - u_I, u_i \rangle = \left\langle v - \sum_{j \in I} c_j u_j, u_i \right\rangle
= \langle v, u_i \rangle - \sum_{j \in I} c_j \langle u_j, u_i \rangle
= \langle v, u_i \rangle - \sum_{j \in I} c_j \|u_i\|^2
= \langle v, u_i \rangle - \langle v, u_i \rangle = 0,
\]
since \( \langle u_j, u_i \rangle = 0 \) for all \( i \neq j \) and \( c_i = \langle v, u_i \rangle / \| u_i \|^2 \). As a consequence, we have

\[
\| v \|^2 = \left\| v - \sum_{i \in I} c_i u_i + \sum_{i \in I} c_i u_i \right\|^2
\]

\[
= \left\| v - \sum_{i \in I} c_i u_i \right\|^2 + \sum_{i \in I} |c_i|^2.
\]

since the \( u_i \) are pairwise orthogonal, that is,

\[
\| v \|^2 = \left\| v - \sum_{i \in I} c_i u_i \right\|^2 + \sum_{i \in I} |c_i|^2.
\]

Thus,

\[
\sum_{i \in I} |c_i|^2 \leq \| v \|^2,
\]

as claimed.

(2) We prove the chain of implications \((a) \Rightarrow (b) \Rightarrow (c) \Rightarrow (a)\).

\((a) \Rightarrow (b)\): If \( v \in V \), since \( V \) is the closure of the subspace spanned by \( (u_k)_{k \in K} \), for every \( \epsilon > 0 \), there is some finite subset \( I \) of \( K \) and some family \( (\lambda_i)_{i \in I} \) of complex numbers, such that

\[
\left\| v - \sum_{i \in I} \lambda_i u_i \right\| < \epsilon.
\]

Now, for every finite subset \( J \) of \( K \) such that \( I \subseteq J \), we have

\[
\left\| v - \sum_{i \in I} \lambda_i u_i \right\|^2 = \left\| v - \sum_{j \in J} c_j u_j + \sum_{j \in J} c_j u_j - \sum_{i \in I} \lambda_i u_i \right\|^2
\]

\[
= \left\| v - \sum_{j \in J} c_j u_j \right\|^2 + \sum_{j \in J} \left| c_j \right|^2 - \sum_{i \in I} \lambda_i |u_i|^2,
\]

since \( I \subseteq J \) and the \( u_j \) (with \( j \in J \)) are orthogonal to \( v - \sum_{j \in J} c_j u_j \) by the argument in (1), which shows that

\[
\left\| v - \sum_{j \in J} c_j u_j \right\| \leq \left\| v - \sum_{i \in I} \lambda_i u_i \right\| < \epsilon,
\]

and thus, that the family \((c_k u_k)_{k \in K}\) is summable with sum \( v \), so that

\[
v = \sum_{k \in K} c_k u_k.
\]
(b) ⇒ (c): If \( v = \sum_{k \in K} c_k u_k \), then for every \( \epsilon > 0 \), there some finite subset \( I \) of \( K \), such that
\[
\left\| v - \sum_{j \in J} c_j u_j \right\| < \sqrt{\epsilon},
\]
for every finite subset \( J \) of \( K \) such that \( I \subseteq J \), and since we proved in (1) that
\[
\|v\|^2 = \left\| v - \sum_{j \in J} c_j u_j \right\|^2 + \sum_{j \in J} |c_j|^2,
\]
we get
\[
\|v\|^2 - \sum_{j \in J} |c_j|^2 < \epsilon,
\]
which proves that \((|c_k|^2)_{k \in K}\) is summable with sum \( \|v\|^2 \).

(c) ⇒ (a): Finally, if \((|c_k|^2)_{k \in K}\) is summable with sum \( \|v\|^2 \), for every \( \epsilon > 0 \), there is some finite subset \( I \) of \( K \) such that
\[
\|v\|^2 - \sum_{j \in J} |c_j|^2 < \epsilon^2
\]
for every finite subset \( J \) of \( K \) such that \( I \subseteq J \), and again, using the fact that
\[
\|v\|^2 = \left\| v - \sum_{j \in J} c_j u_j \right\|^2 + \sum_{j \in J} |c_j|^2,
\]
we get
\[
\left\| v - \sum_{j \in J} c_j u_j \right\| < \epsilon,
\]
which proves that \((c_k u_k)_{k \in K}\) is summable with sum \( \sum_{k \in K} c_k u_k = v \), and \( v \in V \).

(3) Since \( \sum_{i \in I} |c_i|^2 \leq \|v\|^2 \) for every finite subset \( I \) of \( K \), by Proposition A.1, the family \((|c_k|^2)_{k \in K}\) is summable. The Bessel inequality
\[
\sum_{k \in K} |c_k|^2 \leq \|v\|^2
\]
is an obvious consequence of the inequality \( \sum_{i \in I} |c_i|^2 \leq \|v\|^2 \) (for every finite \( I \subseteq K \)). Now, for every natural number \( n \geq 1 \), if \( K_n \) is the subset of \( K \) consisting of all \( c_k \) such that \( |c_k| \geq 1/n \), the number of elements in \( K_n \) is at most
\[
\sum_{k \in K_n} |nc_k|^2 \leq n^2 \sum_{k \in K} |c_k|^2 \leq n^2 \|v\|^2,
\]
which is finite, and thus, at most a countable number of the \( c_k \) may be nonzero.
Since \(|c_k|^2\) is summable with sum \(c\), for every \(\epsilon > 0\), there is some finite subset \(I\) of \(K\) such that
\[
\sum_{j \in J} |c_j|^2 < \epsilon^2
\]
for every finite subset \(J\) of \(K\) such that \(I \cap J = \emptyset\). Since
\[
\left\| \sum_{j \in J} c_j u_j \right\|^2 = \sum_{j \in J} |c_j|^2,
\]
we get
\[
\left\| \sum_{j \in J} c_j u_j \right\| < \epsilon.
\]
This proves that \((c_k u_k)_{k \in K}\) is a Cauchy family, which, by Proposition A.1, implies that \((c_k u_k)_{k \in K}\) is summable, since \(E\) is complete. Thus, the Fourier series \(\sum_{k \in K} c_k u_k\) is summable, with its sum denoted \(u \in V\).

Since \(\sum_{k \in K} c_k u_k\) is summable with sum \(u\), for every \(\epsilon > 0\), there is some finite subset \(I_1\) of \(K\) such that
\[
\left\| u - \sum_{j \in J} c_j u_j \right\| < \epsilon
\]
for every finite subset \(J\) of \(K\) such that \(I_1 \subseteq J\). By the triangle inequality, for every finite subset \(I\) of \(K\),
\[
\left\| u - v \right\| \leq \left\| u - \sum_{i \in I} \lambda_i u_i \right\| + \left\| \sum_{i \in I} \lambda_i u_i - v \right\|.
\]
By (2), every \(w \in V\) is the sum of its Fourier series \(\sum_{k \in K} \lambda_k u_k\), and for every \(\epsilon > 0\), there is some finite subset \(I_2\) of \(K\) such that
\[
\left\| w - \sum_{j \in J} \lambda_j u_j \right\| < \epsilon
\]
for every finite subset \(J\) of \(K\) such that \(I_2 \subseteq J\). By the triangle inequality, for every finite subset \(I\) of \(K\),
\[
\left\| v - \sum_{i \in I} \lambda_i u_i \right\| \leq \left\| v - w \right\| + \left\| w - \sum_{i \in I} \lambda_i u_i \right\|.
\]
Letting \(I = I_1 \cup I_2\), since we showed in (2) that
\[
\left\| v - \sum_{i \in I} c_i u_i \right\| \leq \left\| v - \sum_{i \in I} \lambda_i u_i \right\|
\]
for every finite subset \( I \) of \( K \), we get
\[
\| u - v \| \leq \left( \sum_{i \in I} |c_i u_i| \right) + \sum_{i \in I} |\lambda_i - \lambda_j| u_i \nu_i - v \| \\
\leq \left( \sum_{i \in I} |c_i u_i| \right) + \sum_{i \in I} |\lambda_i u_i - v \| \\
\leq \left( \sum_{i \in I} |c_i u_i| \right) + \| v - w \| + \| w - \sum_{i \in I} \lambda_i u_i \| ,
\]
and thus
\[
\| u - v \| \leq \| v - w \| + 2\epsilon.
\]
Since this holds for every \( \epsilon > 0 \), we have
\[
\| u - v \| \leq \| v - w \|
\]
for all \( w \in V \), i.e. \( \| v - u \| = d(v, V) \), with \( u \in V \), which proves that \( u = p_V(v) \).

A.2 The Hilbert Space \( l^2(K) \) and the Riesz-Fischer Theorem

Proposition A.2 suggests looking at the space of sequences \((z_k)_{k \in K}\) (where \( z_k \in \mathbb{C} \)) such that \((|z_k|^2)_{k \in K}\) is summable. Indeed, such spaces are Hilbert spaces, and it turns out that every Hilbert space is isomorphic to one of those. Such spaces are the infinite-dimensional version of the spaces \( \mathbb{C}^n \) under the usual Euclidean norm.

**Definition A.3.** Given any nonempty index set \( K \), the space \( l^2(K) \) is the set of all sequences \((z_k)_{k \in K}\), where \( z_k \in \mathbb{C} \), such that \((|z_k|^2)_{k \in K}\) is summable, i.e., \( \sum_{k \in K} |z_k|^2 < \infty \).

**Remarks:**

1. When \( K \) is a finite set of cardinality \( n \), \( l^2(K) \) is isomorphic to \( \mathbb{C}^n \).

2. When \( K = \mathbb{N} \), the space \( l^2(\mathbb{N}) \) corresponds to the space \( l^2 \) of Example 2 in Section 12.1 (Vol. I). In that example, we claimed that \( l^2 \) was a Hermitian space, and in fact, a Hilbert space. We now prove this fact for any index set \( K \).

**Proposition A.3.** Given any nonempty index set \( K \), the space \( l^2(K) \) is a Hilbert space under the Hermitian product
\[
\langle (x_k)_{k \in K}, (y_k)_{k \in K} \rangle = \sum_{k \in K} x_k \overline{y}_k.
\]
The subspace consisting of sequences \((z_k)_{k \in K}\) such that \( z_k = 0 \), except perhaps for finitely many \( k \), is a dense subspace of \( l^2(K) \).
Proof. First, we need to prove that \( l^2(K) \) is a vector space. Assume that \((x_k)_{k \in K} \) and \((y_k)_{k \in K} \) are in \( l^2(K) \). This means that \(|x_k|^2\) and \(|y_k|^2\) are summable, which, in view of Proposition A.1, is equivalent to the existence of some positive bounds \( A \) and \( B \) such that \( \sum_{i \in I} |x_i|^2 < A \) and \( \sum_{i \in I} |y_i|^2 < B \), for every finite subset \( I \) of \( K \). To prove that \((|x_k + y_k|^2)_{k \in K} \) is summable, it is sufficient to prove that there is some \( C > 0 \) such that \( \sum_{i \in I} |x_i + y_i|^2 < C \) for every finite subset \( I \) of \( K \). However, the parallelogram inequality implies that

\[
\sum_{i \in I} |x_i + y_i|^2 \leq \sum_{i \in I} 2(|x_i|^2 + |y_i|^2) \leq 2(A + B),
\]

for every finite subset \( I \) of \( K \), and we conclude by Proposition A.1. Similarly, for every \( \lambda \in \mathbb{C} \),

\[
\sum_{i \in I} |\lambda x_i|^2 \leq \sum_{i \in I} |\lambda|^2 |x_i|^2 \leq |\lambda|^2 A,
\]

and \((\lambda_k x_k)_{k \in K} \) is summable. Therefore, \( l^2(K) \) is a vector space.

By the Cauchy-Schwarz inequality,

\[
\sum_{i \in I} |x_i y_i| \leq \sum_{i \in I} |x_i| |y_i| \leq \left( \sum_{i \in I} |x_i|^2 \right)^{1/2} \left( \sum_{i \in I} |y_i|^2 \right)^{1/2} \leq \sum_{i \in I} (|x_i|^2 + |y_i|^2)/2 \leq (A + B)/2,
\]

for every finite subset \( I \) of \( K \). Here, we used the fact that

\[
4CD \leq (C + D)^2,
\]

which is equivalent to

\[
(C - D)^2 \geq 0.
\]

By Proposition A.1, \((|x_k y_k|)_{k \in K} \) is summable. The customary language is that \((x_k y_k)_{k \in K} \) is absolutely summable. However, it is a standard fact that this implies that \((x_k y_k)_{k \in K} \) is summable (For every \( \epsilon > 0 \), there is some finite subset \( I \) of \( K \) such that

\[
\sum_{j \in J} |x_j y_j| < \epsilon
\]

for every finite subset \( J \) of \( K \) such that \( I \cap J = \emptyset \), and thus

\[
|\sum_{j \in J} x_j y_j| \leq \sum_{i \in J} |x_j y_j| < \epsilon,
\]

proving that \((x_k y_k)_{k \in K} \) is a Cauchy family, and thus summable). We still have to prove that \( l^2(K) \) is complete.

Consider a sequence \((\lambda_k^n)_{n \geq 1} \) of sequences \((\lambda_k^n)_{k \in K} \in l^2(K) \), and assume that it is a Cauchy sequence. This means that for every \( \epsilon > 0 \), there is some \( N \geq 1 \) such that

\[
\sum_{k \in K} |\lambda_k^m - \lambda_k^n|^2 < \epsilon^2
\]
for all \( m, n \geq N \). For every fixed \( k \in K \), this implies that
\[
|\lambda^n_k - \lambda^n_m| < \epsilon
\]
for all \( m, n \geq N \), which shows that \((\lambda^n_k)_{n \geq 1}\) is a Cauchy sequence in \( \mathbb{C} \). Since \( \mathbb{C} \) is complete, the sequence \((\lambda^n_k)_{n \geq 1}\) has a limit \( \lambda_k \in \mathbb{C} \). We claim that \((\lambda_k)_{k \in K} \in l^2(K)\) and that this is the limit of \((((\lambda^n_k)_{k \in K})_{n \geq 1}\). Given any \( \epsilon > 0 \), the fact that \((((\lambda^n_k)_{k \in K})_{n \geq 1}\) is a Cauchy sequence implies that there is some \( N \geq 1 \) such that for every finite subset \( I \) of \( K \), we have
\[
\sum_{i \in I} |\lambda^n_i - \lambda^n_m|^2 < \epsilon/4
\]
for all \( m, n \geq N \). Let \( p = |I| \). Then,
\[
|\lambda^n_i - \lambda^n_m| < \frac{\sqrt{\epsilon}}{2\sqrt{p}}
\]
for every \( i \in I \). Since \( \lambda_i \) is the limit of \((\lambda^n_i)_{n \geq 1}\), we can find some \( n \) large enough so that
\[
|\lambda^n_i - \lambda_i| < \frac{\sqrt{\epsilon}}{2\sqrt{p}}
\]
for every \( i \in I \). Since
\[
|\lambda^n_i - \lambda_i| \leq |\lambda^n_i - \lambda^n_m| + |\lambda^n_m - \lambda_i|,
\]
we get
\[
|\lambda^n_i - \lambda_i| < \frac{\sqrt{\epsilon}}{\sqrt{p}},
\]
and thus,
\[
\sum_{i \in I} |\lambda^n_i - \lambda_i|^2 < \epsilon,
\]
for all \( m \geq N \). Since the above holds for every finite subset \( I \) of \( K \), by Proposition A.1, we get
\[
\sum_{k \in K} |\lambda^m_k - \lambda_k|^2 < \epsilon,
\]
for all \( m \geq N \). This proves that \((\lambda^m_k - \lambda_k)_{k \in K} \in l^2(K)\) for all \( m \geq N \), and since \( l^2(K) \) is a vector space and \((\lambda^m_k)_{k \in K} \in l^2(K)\) for all \( m \geq 1 \), we get \((\lambda_k)_{k \in K} \in l^2(K)\). However,
\[
\sum_{k \in K} |\lambda^m_k - \lambda_k|^2 < \epsilon
\]
for all \( m \geq N \), means that the sequence \((\lambda^m_k)_{k \in K}\) converges to \((\lambda_k)_{k \in K} \in l^2(K)\). The fact that the subspace consisting of sequences \((z_k)_{k \in K}\) such that \( z_k = 0 \) except perhaps for finitely many \( k \) is a dense suspace of \( l^2(K) \) is left as an easy exercise. \( \square \)
Remark: The subspace consisting of all sequences \( (z_k)_{k \in K} \) such that \( z_k = 0 \), except perhaps for finitely many \( k \), provides an example of a subspace which is not closed in \( l^2(K) \). Indeed, this space is strictly contained in \( l^2(K) \), since there are countable sequences of nonnull elements in \( l^2(K) \) (why?).

We just need two more propositions before being able to prove that every Hilbert space is isomorphic to some \( l^2(K) \).

**Proposition A.4.** Let \( E \) be a Hilbert space, and \( (u_k)_{k \in K} \) an orthogonal family in \( E \). The following properties hold:

1. For every family \( (\lambda_k)_{k \in K} \in l^2(K) \), the family \( (\lambda_k u_k)_{k \in K} \) is summable. Furthermore, \( v = \sum_{k \in K} \lambda_k u_k \) is the only vector such that \( c_k = \lambda_k \) for all \( k \in K \), where the \( c_k \) are the Fourier coefficients of \( v \).

2. For any two families \( (\lambda_k)_{k \in K} \in l^2(K) \) and \( (\mu_k)_{k \in K} \in l^2(K) \), if \( v = \sum_{k \in K} \lambda_k u_k \) and \( w = \sum_{k \in K} \mu_k u_k \), we have the following equation, also called Parseval identity:

\[
\langle v, w \rangle = \sum_{k \in K} \lambda_k \mu_k.
\]

**Proof.** (1) The fact that \( (\lambda_k)_{k \in K} \in l^2(K) \) means that \( (|\lambda_k|^2)_{k \in K} \) is summable. The proof given in Proposition A.2 (3) applies to the family \( (|\lambda_k|^2)_{k \in K} \) (instead of \( (|c_k|^2)_{k \in K} \)), and yields the fact that \( (\lambda_k u_k)_{k \in K} \) is summable. Letting \( v = \sum_{k \in K} \lambda_k u_k \), recall that \( c_k = \langle v, u_k \rangle / \| u_k \|^2 \).

Pick some \( k \in K \). Since \( \langle -, - \rangle \) is continuous, for every \( \epsilon > 0 \), there is some \( \eta > 0 \) such that

\[
|\langle v, u_k \rangle - \langle w, u_k \rangle| < \epsilon \| u_k \|^2
\]

whenever \( \| v - w \| < \eta \).

However, since for every \( \eta > 0 \), there is some finite subset \( I \) of \( K \) such that

\[
\left\| v - \sum_{j \in J} \lambda_j u_j \right\| < \eta
\]

for every finite subset \( J \) of \( K \) such that \( I \subseteq J \), we can pick \( J = I \cup \{k\} \), and letting \( w = \sum_{j \in J} \lambda_j u_j \), we get

\[
|\langle v, u_k \rangle - \left\langle \sum_{j \in J} \lambda_j u_j, u_k \right\rangle| < \epsilon \| u_k \|^2.
\]

However,

\[
\langle v, u_k \rangle = c_k \| u_k \|^2 \quad \text{and} \quad \left\langle \sum_{j \in J} \lambda_j u_j, u_k \right\rangle = \lambda_k \| u_k \|^2,
\]

and thus, the above proves that \( |c_k - \lambda_k| < \epsilon \) for every \( \epsilon > 0 \), and thus, that \( c_k = \lambda_k \).
A.2. **THE HILBERT SPACE** $l^2(K)$ **AND THE RIESZ-FISCHER THEOREM**

(2) Since $\langle -, - \rangle$ is continuous, for every $\epsilon > 0$, there are some $\eta_1 > 0$ and $\eta_2 > 0$, such that

$$|\langle x, y \rangle| < \epsilon$$

whenever $\|x\| < \eta_1$ and $\|y\| < \eta_2$. Since $v = \sum_{k \in K} \lambda_k u_k$ and $w = \sum_{k \in K} \mu_k u_k$, there is some finite subset $I_1$ of $K$ such that

$$\|v - \sum_{j \in J} \lambda_j u_j\| < \eta_1$$

for every finite subset $J$ of $K$ such that $I_1 \subseteq J$, and there is some finite subset $I_2$ of $K$ such that

$$\|w - \sum_{j \in J} \mu_j u_j\| < \eta_2$$

for every finite subset $J$ of $K$ such that $I_2 \subseteq J$. Letting $I = I_1 \cup I_2$, we get

$$\left| \langle v - \sum_{i \in I} \lambda_i u_i, w - \sum_{i \in I} \mu_i u_i \rangle \right| < \epsilon.$$ 

Furthermore,

$$\langle v, w \rangle = \langle v - \sum_{i \in I} \lambda_i u_i + \sum_{i \in I} \lambda_i u_i, w - \sum_{i \in I} \mu_i u_i + \sum_{i \in I} \mu_i u_i \rangle$$

$$= \langle v - \sum_{i \in I} \lambda_i u_i, w - \sum_{i \in I} \mu_i u_i \rangle + \sum_{i \in I} \lambda_i \overline{\mu_i},$$

since the $u_i$ are orthogonal to $v - \sum_{i \in I} \lambda_i u_i$ and $w - \sum_{i \in I} \mu_i u_i$ for all $i \in I$. This proves that for every $\epsilon > 0$, there is some finite subset $I$ of $K$ such that

$$\left| \langle v, w \rangle - \sum_{i \in I} \lambda_i \overline{\mu_i} \right| < \epsilon.$$ 

We already know from Proposition A.3 that $(\lambda_k \overline{\mu_k})_{k \in K}$ is summable, and since $\epsilon > 0$ is arbitrary, we get

$$\langle v, w \rangle = \sum_{k \in K} \lambda_k \overline{\mu_k}.$$ 


The next proposition states properties characterizing Hilbert bases (total orthogonal families).

**Proposition A.5.** Let $E$ be a Hilbert space, and let $(u_k)_{k \in K}$ be an orthogonal family in $E$. The following properties are equivalent:
(1) The family \((u_k)_{k \in K}\) is a total orthogonal family.

(2) For every vector \(v \in E\), if \((c_k)_{k \in K}\) are the Fourier coefficients of \(v\), then the family \((c_k u_k)_{k \in K}\) is summable and \(v = \sum_{k \in K} c_k u_k\).

(3) For every vector \(v \in E\), we have the Parseval identity:
\[
\|v\|^2 = \sum_{k \in K} |c_k|^2.
\]

(4) For every vector \(u \in E\), if \(\langle u, u_k \rangle = 0\) for all \(k \in K\), then \(u = 0\).

Proof. The equivalence of (1), (2), and (3), is an immediate consequence of Proposition A.2 and Proposition A.4.

(4) If \((u_k)_{k \in K}\) is a total orthogonal family and \(\langle u, u_k \rangle = 0\) for all \(k \in K\), since \(u = \sum_{k \in K} c_k u_k\) where \(c_k = \langle u, u_k \rangle / \|u_k\|^2\), we have \(c_k = 0\) for all \(k \in K\), and \(u = 0\).

Conversely, assume that the closure \(V\) of \((u_k)_{k \in K}\) is different from \(E\). Then, by Proposition 29.7, we have \(E = V \oplus V^\perp\), where \(V^\perp\) is the orthogonal complement of \(V\), and \(V^\perp\) is nontrivial since \(V \neq E\). As a consequence, there is some nonnull vector \(u \in V^\perp\). But then, \(u\) is orthogonal to every vector in \(V\), and in particular,
\[
\langle u, u_k \rangle = 0
\]
for all \(k \in K\), which, by assumption, implies that \(u = 0\), contradicting the fact that \(u \neq 0\).

Remarks:

(1) If \(E\) is a Hilbert space and \((u_k)_{k \in K}\) is a total orthogonal family in \(E\), there is a simpler argument to prove that \(u = 0\) if \(\langle u, u_k \rangle = 0\) for all \(k \in K\), based on the continuity of \(\langle -, - \rangle\). The argument is to prove that the assumption implies that \(\langle v, u \rangle = 0\) for all \(v \in E\). Since \(\langle -, - \rangle\) is positive definite, this implies that \(u = 0\). By continuity of \(\langle -, - \rangle\), for every \(\epsilon > 0\), there is some \(\eta > 0\) such that for every finite subset \(I\) of \(K\), for every family \((\lambda_i)_{i \in I}\), for every \(v \in E\),
\[
\left| \langle v, u \rangle - \left\langle \sum_{i \in I} \lambda_i u_i, u \right\rangle \right| < \epsilon
\]
whenever
\[
\left\| v - \sum_{i \in I} \lambda_i u_i \right\| < \eta.
\]
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Since $(u_k)_{k \in K}$ is dense in $E$, for every $v \in E$, there is some finite subset $I$ of $K$ and some family $(\lambda_i)_{i \in I}$ such that

$$\left\| v - \sum_{i \in I} \lambda_i u_i \right\| < \eta,$$

and since by assumption, $\langle \sum_{i \in I} \lambda_i u_i, u \rangle = 0$, we get

$$|\langle v, u \rangle| < \epsilon.$$

Since this holds for every $\epsilon > 0$, we must have $\langle v, u \rangle = 0$.

(2) If $V$ is any nonempty subset of $E$, the kind of argument used in the previous remark can be used to prove that $V^\perp$ is closed (even if $V$ is not), and that $V^\perp\perp$ is the closure of $V$.

We will now prove that every Hilbert space has some Hilbert basis. This requires using a fundamental theorem from set theory known as Zorn’s Lemma, which we quickly review.

Given any set $X$ with a partial ordering $\leq$, recall that a nonempty subset $C$ of $X$ is a chain if it is totally ordered (i.e., for all $x, y \in C$, either $x \leq y$ or $y \leq x$). A nonempty subset $Y$ of $X$ is bounded iff there is some $b \in X$ such that $y \leq b$ for all $y \in Y$. Some $m \in X$ is maximal iff for every $x \in X$, $m \leq x$ implies that $x = m$. We can now state Zorn’s Lemma. For more details, see Rudin [83], Lang [63], or Artin [6].

**Proposition A.6.** Given any nonempty partially ordered set $X$, if every (nonempty) chain in $X$ is bounded, then $X$ has some maximal element.

We can now prove the existence of Hilbert bases. We define a partial order on families $(u_k)_{k \in K}$ as follows: For any two families $(u_k)_{k \in K_1}$ and $(v_k)_{k \in K_2}$, we say that

$$(u_k)_{k \in K_1} \leq (v_k)_{k \in K_2}$$

iff $K_1 \subseteq K_2$ and $u_k = v_k$ for all $k \in K_1$. This is clearly a partial order.

**Proposition A.7.** Let $E$ be a Hilbert space. Given any orthogonal family $(u_k)_{k \in K}$ in $E$, there is a total orthogonal family $(u_l)_{l \in L}$ containing $(u_k)_{k \in K}$.

**Proof.** Consider the set $\mathcal{S}$ of all orthogonal families greater than or equal to the family $B = (u_k)_{k \in K}$. We claim that every chain in $\mathcal{S}$ is bounded. Indeed, if $C = (C_l)_{l \in L}$ is a chain in $\mathcal{S}$, where $C_l = (u_{k,l})_{k \in K_l}$, the union family

$$(u_k)_{k \in \bigcup_{l \in L} K_l}, \text{ where } u_k = u_{k,l} \text{ whenever } k \in K_l,$$

is clearly an upper bound for $C$, and it is immediately verified that it is an orthogonal family. By Zorn’s Lemma A.6, there is a maximal family $(u_l)_{l \in L}$ containing $(u_k)_{k \in K}$. If $(u_l)_{l \in L}$ is not dense in $E$, then its closure $V$ is strictly contained in $E$, and by Proposition 29.7, the
orthogonal complement $V^\perp$ of $V$ is nontrivial since $V \neq E$. As a consequence, there is some nonnull vector $u \in V^\perp$. But then, $u$ is orthogonal to every vector in $(u_l)_{l \in L}$, and we can form an orthogonal family strictly greater than $(u_l)_{l \in L}$ by adding $u$ to this family, contradicting the maximality of $(u_l)_{l \in L}$. Therefore, $(u_l)_{l \in L}$ is dense in $E$, and thus, it is a Hilbert basis. □

Remark: It is possible to prove that all Hilbert bases for a Hilbert space $E$ have index sets $K$ of the same cardinality. For a proof, see Bourbaki [21].

Definition A.4. A Hilbert space $E$ is separable if its Hilbert bases are countable.

At last, we can prove that every Hilbert space is isomorphic to some Hilbert space $l^2(K)$ for some suitable $K$.

Theorem A.8. (Riesz-Fischer) For every Hilbert space $E$, there is some nonempty set $K$ such that $E$ is isomorphic to the Hilbert space $l^2(K)$. More specifically, for any Hilbert basis $(u_k)_{k \in K}$ of $E$, the maps $f : l^2(K) \to E$ and $g : E \to l^2(K)$ defined such that

$$f((\lambda_k)_{k \in K}) = \sum_{k \in K} \lambda_k u_k \quad \text{and} \quad g(u) = \left(\langle u, u_k \rangle/\|u_k\|^2\right)_{k \in K} = (c_k)_{k \in K},$$

are bijective linear isometries such that $g \circ f = \text{id}$ and $f \circ g = \text{id}$.

Proof. By Proposition A.4 (1), the map $f$ is well defined, and it it clearly linear. By Proposition A.2 (3), the map $g$ is well defined, and it is also clearly linear. By Proposition A.2 (2b), we have

$$f(g(u)) = u = \sum_{k \in K} c_k u_k,$$

and by Proposition A.4 (1), we have

$$g(f((\lambda_k)_{k \in K})) = (\lambda_k)_{k \in K},$$

and thus $g \circ f = \text{id}$ and $f \circ g = \text{id}$. By Proposition A.4 (2), the linear map $g$ is an isometry. Therefore, $f$ is a linear bijection and an isometry between $l^2(K)$ and $E$, with inverse $g$. □

Remark: The surjectivity of the map $g : E \to l^2(K)$ is known as the Riesz-Fischer theorem.

Having done all this hard work, we sketch how these results apply to Fourier series. Again, we refer the readers to Rudin [83] or Lang [65, 66] for a comprehensive exposition.

Let $C(T)$ denote the set of all periodic continuous functions $f : [-\pi, \pi] \to \mathbb{C}$ with period $2\pi$. There is a Hilbert space $L^2(T)$ containing $C(T)$ and such that $C(T)$ is dense in $L^2(T)$, whose inner product is given by

$$\langle f, g \rangle = \int_{-\pi}^\pi f(x)\overline{g(x)}dx.$$
The Hilbert space $L^2(T)$ is the space of Lebesgue square-integrable periodic functions (of period $2\pi$).

It turns out that the family $(e^{ikx})_{k \in \mathbb{Z}}$ is a total orthogonal family in $L^2(T)$, because it is already dense in $C(T)$ (for instance, see Rudin [83]). Then, the Riesz-Fischer theorem says that for every family $(c_k)_{k \in \mathbb{Z}}$ of complex numbers such that
\[ \sum_{k \in \mathbb{Z}} |c_k|^2 < \infty, \]
there is a unique function $f \in L^2(T)$ such that $f$ is equal to its Fourier series
\[ f(x) = \sum_{k \in \mathbb{Z}} c_k e^{ikx}, \]
where the Fourier coefficients $c_k$ of $f$ are given by the formula
\[ c_k = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(t) e^{-ikt} dt. \]

The Parseval theorem says that
\[ \sum_{k=-\infty}^{+\infty} c_k d_k = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(t) \overline{g(t)} dt \]
for all $f, g \in L^2(T)$, where $c_k$ and $d_k$ are the Fourier coefficients of $f$ and $g$.

Thus, there is an isomorphism between the two Hilbert spaces $L^2(T)$ and $l^2(\mathbb{Z})$, which is the deep reason why the Fourier coefficients “work”. Theorem A.8 implies that the Fourier series $\sum_{k \in \mathbb{Z}} c_k e^{ikx}$ of a function $f \in L^2(T)$ converges to $f$ in the $L^2$-sense, i.e., in the mean-square sense. This does not necessarily imply that the Fourier series converges to $f$ pointwise! This is a subtle issue, and for more on this subject, the reader is referred to Lang [65, 66] or Schwartz [93, 94].

We can also consider the set $C([-1, 1])$ of continuous functions $f : [-1, 1] \to \mathbb{C}$. There is a Hilbert space $L^2([-1, 1])$ containing $C([-1, 1])$ and such that $C([-1, 1])$ is dense in $L^2([-1, 1])$, whose inner product is given by
\[ \langle f, g \rangle = \int_{-1}^{1} f(x) g(x) dx. \]

The Hilbert space $L^2([-1, 1])$ is the space of Lebesgue square-integrable functions over $[-1, 1]$. The Legendre polynomials $P_n(x)$ defined in Example 5 of Section 10.2 (Chapter 10, Vol. I) form a Hilbert basis of $L^2([-1, 1])$. Recall that if we let $f_n$ be the function
\[ f_n(x) = (x^2 - 1)^n, \]
$P_n(x)$ is defined as follows:

$$P_0(x) = 1, \quad \text{and} \quad P_n(x) = \frac{1}{2^n n!} f_n^{(n)}(x),$$

where $f_n^{(n)}$ is the $n$th derivative of $f_n$. The reason for the leading coefficient is to get

$$P_n(1) = 1.$$  

It can be shown with much efforts that

$$P_n(x) = \sum_{0 \leq k \leq n/2} (-1)^k \frac{(2(n-k))!}{2^n(n-k)!k!(n-2k)!} x^{n-2k}.$$
Bibliography


