Optimization Problem

 $\begin{array}{ll} \text{Minimize} & f(\mathbf{w}, b) \equiv \frac{1}{2} \|\mathbf{w}\|^2 \\ \text{subject to} & y_i(\mathbf{w} \cdot \mathbf{x}_i + b) \geq 1, \quad i = 1, \dots, m \end{array}$

This is an optimization problem in (n + 1) variables, with m linear inequality constraints.

Introducing Lagrange multipliers α_i , i = 1, ..., m for the inequality constraints above gives the primal Lagrangian:

$$\begin{array}{ll} \text{Minimize} & L_P(\mathbf{w}, b, \alpha) \equiv \frac{1}{2} \|\mathbf{w}\|^2 - \sum_{i=1}^m \alpha_i [y_i(\mathbf{w} \cdot \mathbf{x}_i + b) - 1] \\ \text{subject to} & \alpha_i \geq 0, \quad i = 1, \dots, m \end{array}$$

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Optimization Problem (continued)

Setting the gradients of L_P with respect to \mathbf{w}, b equal to zero gives:

$$\frac{\partial L_P}{\partial \mathbf{w}} = \mathbf{0} \Rightarrow \mathbf{w} = \sum_{i=1}^m \alpha_i y_i \mathbf{x}_i, \quad \frac{\partial L_P}{\partial b} = \mathbf{0} \Rightarrow \sum_{i=1}^m \alpha_i y_i = \mathbf{0}$$

Substituting the above in the primal gives the following dual problem:

Maximize
$$L_D(\alpha) \equiv \sum_{i=1}^m \alpha_i - \frac{1}{2} \sum_{i,j=1}^m \alpha_i \alpha_j y_i y_j (\mathbf{x}_i \cdot \mathbf{x}_j)$$

subject to $\sum_{i=1}^m \alpha_i y_i = 0; \quad \alpha_i \ge 0, \ i = 1, \dots, m$

This is a convex quadratic programming problem in α .

Solution

The parameters w, b of the maximal margin classifier are determined by the solution α to the dual problem:

$$\mathbf{w} = \sum_{i=1}^{m} \alpha_i y_i \mathbf{x}_i$$
$$b = -\frac{1}{2} \left(\min_{y_i = +1} (\mathbf{w} \cdot \mathbf{x}_i) + \max_{y_i = -1} (\mathbf{w} \cdot \mathbf{x}_i) \right)$$

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Support Vectors

Due to certain properties of the solution (known as the Karush-Kuhn-Tucker conditions), the solution α must satisfy

$$\alpha_i[y_i(\mathbf{w} \cdot \mathbf{x}_i + b) - 1] = 0, \quad i = 1, \dots, m.$$

Thus, $\alpha_i > 0$ only for those points x_i that are closest to the classifying hyperplane. These points are called the **support vectors**.



Non-Separable Case

Want to relax the constraints

$$y_i(\mathbf{w} \cdot \mathbf{x}_i + b) \ge 1.$$

Can introduce slack variables ξ_i :

$$y_i(\mathbf{w} \cdot \mathbf{x}_i + b) \ge 1 - \xi_i,$$

where $\xi_i \ge 0 \ \forall i$. An error occurs when $\xi_i > 1$.

Thus we can assign an extra cost for errors as follows:

Minimize
$$f(\mathbf{w}, b, \boldsymbol{\xi}) \equiv \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{i=1}^m \xi_i$$

subject to $y_i(\mathbf{w} \cdot \mathbf{x}_i + b) \ge 1 - \xi_i; \quad \xi_i \ge 0, \quad i = 1, \dots, m$

Non-Separable Case (continued)

Dual problem:

Maximize
$$L_D(\boldsymbol{\alpha}) \equiv \sum_{i=1}^m \alpha_i - \frac{1}{2} \sum_{i,j=1}^m \alpha_i \alpha_j y_i y_j (\mathbf{x}_i \cdot \mathbf{x}_j)$$

subject to $\sum_{i=1}^m \alpha_i y_i = 0; \quad 0 \le \alpha_i \le C, \quad i = 1, \dots, m$

Solution:

The solution for \mathbf{w} is again given by

$$\mathbf{w} = \sum_{i=1}^{m} \alpha_i y_i \mathbf{x}_i.$$

The solution for b is similar to that in the linear case.

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Visualizing the Solution in the Non-Separable Case



- Margin support vectors $\xi_i = 0$ Correct 1.
- Non-margin support vectors $\xi_i < 1$ Correct (in margin) 2.
- 3. Non-margin support vectors $\xi_i > 1$ Error