

Support Vector Machines (SVM)

Dan Roth danroth@seas.upenn.edu|http://www.cis.upenn.edu/~danroth/|461C, 3401 Walnut

Slides were created by Dan Roth (for CIS519/419 at Penn or CS446 at UIUC), and other authors who have made their ML slides available.



Available on the web site

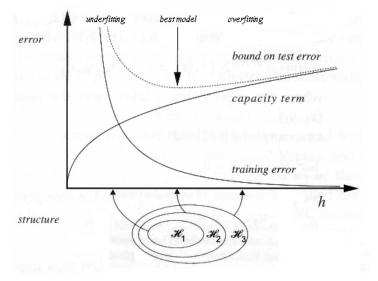
- Remember that all the lectures are available on the website before the class
 - Go over it and be prepared
 - A new set of written notes will accompany most lectures, with some more details, examples and, (when relevant) some code.
- HW 3: Due on 11/16/20
 - You cannot solve all the problems yet.
 - Less time consuming; no programming
- Projects

Projects

- CIS 519 students need to do a team project
 - Teams will be of size 2-4
 - We will help grouping if needed
- There will be 3 projects.
 - Natural Language Processing (Text)
 - Computer Vision (Images)
 - Speech (Audio)
- In all cases, we will give you datasets and initial ideas
 - The problem will be multiclass classification problems
 - You will get annotated data only for some of the labels, but will also have to predict other labels
 - O-zero shot learning; few-shot learning; transfer learning
- A detailed note will come out today.
- Timeline:
 - 11/11 Choose a project and team up
 - 11/23 Initial proposal describing what your team plans to do
 - 12/2 Progress report
 - 12/15-20 (TBD) Final paper + short video
- Try to make it interesting!

COLT approach to explaining Learning

- No Distributional Assumption
- Training Distribution is the same as the Test Distribution
- Generalization bounds depend on this view and affects model selection. $Err_{D}(h) < Err_{TR}(h) + P(VC(H), \log(\frac{1}{\gamma}), \frac{1}{m})$



This is also called the

"Structural Risk Minimization" principle.

COLT approach to explaining Learning

- No Distributional Assumption
- Training Distribution is the same as the Test Distribution
- Generalization bounds depend on this view and affect model selection.

 $Err_D(h) < Err_{TR}(h) + P(VC(H), \log(1/\Upsilon), 1/m)$

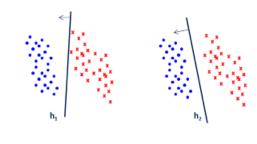
- As presented, the VC dimension is a combinatorial parameter that is associated with a class of functions.
- We know that the class of linear functions has a lower VC dimension than the class of quadratic functions.
 - But this notion can be refined to depend on a given data set, and this way directly affect the hypothesis chosen for a given data set.

Data Dependent VC dimension

- So far, we discussed VC dimension in the context of a <u>fixed</u> class of functions.
- We can also parameterize the class of functions in interesting ways.
- Consider the class of linear functions, parameterized by their margin. Note that this is a data dependent notion.

Linear Classification

- Let $X = R^2, Y = \{+1, -1\}$
- Which of these classifiers would be likely to generalize better?



CIS 419/519 Fall'19

VC and Linear Classification

• Recall the VC based generalization bound:

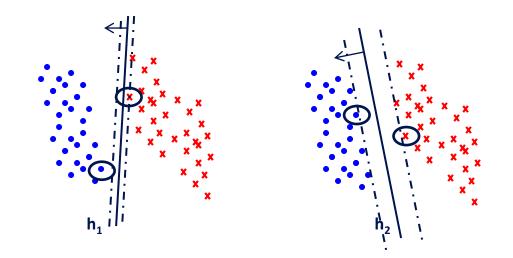
$$Err(h) \leq err_{TR}(h) + Poly\{VC(H), \frac{1}{m}, \log(\frac{1}{\gamma})\}$$

• Here we get the same bound for both classifiers: $Err_{TR}(h_1) = Err_{TR}(h_2) = 0$ $h_1, h_2 \in H_{lin(2)}, VC(H_{lin(2)}) = 3$

• How, then, can we explain our intuition that h_2 should give better generalization than h_1 ?

Linear Classification

• Although both classifiers separate the data, the distance with which the separation is achieved is different:



Concept of Margin

• The margin Υ_i of a point $x_i \in \mathbb{R}^n$ with respect to a linear classifier $h(x) = sign(\mathbf{w}^T \cdot \mathbf{x} + b)$ is defined as the distance of x_i from the hyperplane $\mathbf{w}^T \cdot \mathbf{x} + b = 0$:

$$\Upsilon_i = \left| \frac{\boldsymbol{w}^T \cdot \boldsymbol{x}_i + \boldsymbol{b}}{\|\boldsymbol{w}\|} \right|$$

The margin of <u>a set of points</u> {x₁, ... x_m} with respect to a hyperplane w, is defined as the margin of the point closest to the hyperplane:

$$\Upsilon = \min_{i} \Upsilon_{i} = \min_{i} \left| \frac{\mathbf{w}^{T} \cdot \mathbf{x}_{i} + b}{\|\mathbf{w}\|} \right|$$

VC and Linear Classification

 Theorem: If H_Y is the space of all linear classifiers in **R**ⁿ that separate the training data with margin at least Y, then:

 $VC(H_{\Upsilon}) \leq \min(\frac{R^2}{\gamma^2}, n) + 1,$

In particular, you see here that for "general" linear separators of dimensionality n, the VC is n+1

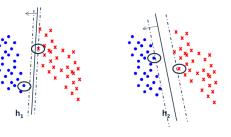
- Where *R* is the radius of the smallest sphere (in *R*^{*n*}) that contains the data.
- Thus, for such classifiers, we have a bound of the form:

$$Err(h) \leq err_{TR}(h) + \left\{\frac{O\left(\frac{R^2}{\gamma^2}\right) + \log\left(\frac{4}{\delta}\right)}{m}\right\}^{1/2}$$

Towards Max Margin Classifiers

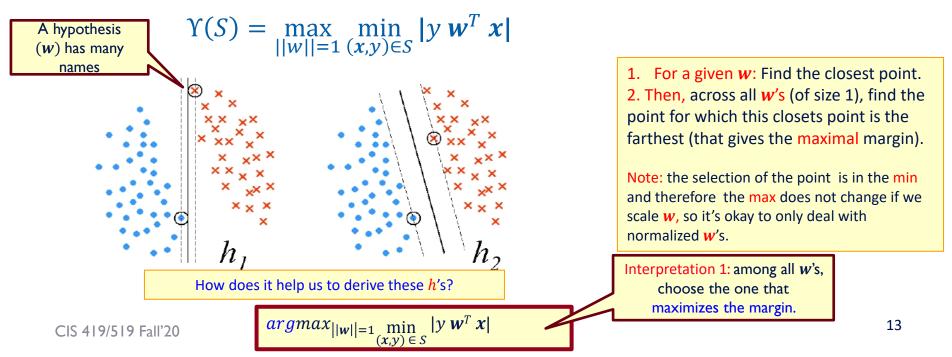
- First observation: When we consider the class H_{Υ} of linear hypotheses that separate a given data set with a margin Υ , we see that
 - Large Margin $\Upsilon \rightarrow$ Small VC dimension of H_{Υ}
- Consequently, our goal could be to find a separating hyperplane *w* that <u>maximizes the margin</u> of the set *S* of examples.
- A second observation that drives an algorithmic approach is that:
 - Small $||w|| \rightarrow$ Large Margin
- Together, this leads to an algorithm: from among all those w's that agree with the data, find the one with the minimal size ||w||
 - But, if w separates the data, so does w/7....
 - We need to better understand the relations between *w* and the margin

But, how can we do it algorithmically?



Maximal Margin

- This discussion motivates the notion of a maximal margin.
- The maximal margin of <u>a data set S</u> is defined as:



Recap: Margin and VC dimension

Believe Theorem (Vapnik): If H_{γ} is the space of all linear classifiers in \mathbb{R}^n that separate the training data with margin at least Υ , then $VC(H_{\gamma}) \leq R^2/\Upsilon^2$

- where R is the radius of the smallest sphere (in \mathbb{R}^n) that contains the data.

- This is the first observation that will lead to an algorithmic approach.
- The second observation is that: Small $||w|| \rightarrow$ Large Margin
- Consequently, the algorithm will be: from among all those *w*'s that agree with the data, find the one with the minimal size ||*w*||

From Margin to ||w||

- We want to choose the hyperplane that achieves the largest margin. That is, given a data set *S*, find:
 - $\boldsymbol{w}^* = \operatorname{argmax}_{||\boldsymbol{w}||=1} \min_{(\boldsymbol{x},\boldsymbol{y})\in S} |\boldsymbol{y} \boldsymbol{w}^T \boldsymbol{x}|$
- How to find this **w***?
- Claim: Define w_0 to be the solution of the optimization problem
 - $w_0 = argmin \{ ||w||^2 : \forall (x, y) \in S, y w^T x \ge 1 \}.$

Interpretation 2: among all *w*'s that separate the data with margin 1, choose the one with minimal size.

- Then:
- $\mathbf{w}_0/||\mathbf{w}_0|| = \operatorname{argmax}_{||\mathbf{w}||=1} \min_{(\mathbf{x}, \mathbf{y}) \in S} y \mathbf{w}^T \mathbf{x}$
- That is, the normalization of w_0 corresponds to the largest margin separating hyperplane.

From Margin to ||w||(2)

$$\boldsymbol{w}^* = \operatorname{argmax}_{||\boldsymbol{w}||=1} \min_{(\boldsymbol{x},\boldsymbol{y})\in S} |\boldsymbol{y} \boldsymbol{w}^T \boldsymbol{x}|$$

And, recall that $\Upsilon(S)$ is the

maximal margin for the set S

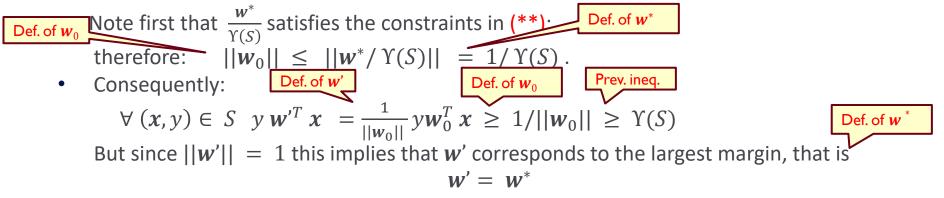
• Claim: Define w_0 to be the solution of the optimization problem:

- $w_0 = argmin\{||w||^2 : \forall (x, y) \in S, y \ w^T x \ge 1\}$ (**) Then:

 $- w_0/||w_0|| = argmax_{||w||=1} \min_{(x,y)\in S} y w^T x$

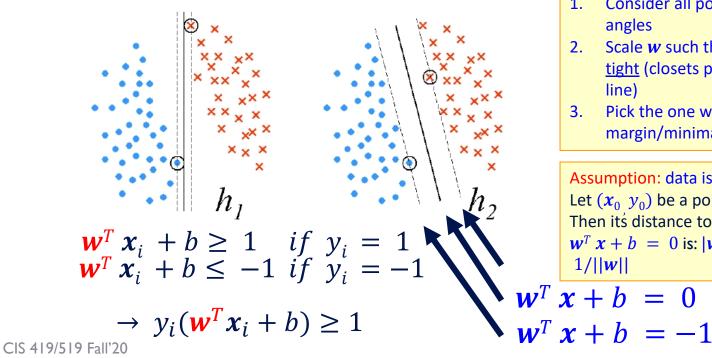
That is, the normalization of w_0 corresponds to the largest margin separating hyperplane.

• Proof: Define $w' = w_0/||w_0||$ and let w^* be the largest-margin separating hyperplane of size 1. We need to show that $w' = w^*$.



Margin of a Separating Hyperplane

• A separating hyperplane: $w^T x + b = 0$



Distance between $w^T x + b = +1 and - 1 is 2/||w||$ What we did:

- Consider all possible *w* with different 1. angles
- 2. Scale *w* such that the constraints are tight (closets points are on the +/-1 line)
- Pick the one with largest 3. margin/minimal size

Assumption: data is linearly separable Let $(\mathbf{x}_0 \ \mathbf{y}_0)$ be a point on $\mathbf{w}^T \mathbf{x} + b = 1$ Then its distance to the separating plane $w^T x + b = 0$ is: $|w^T x_0 + b| / ||w|| =$ 1/||**w**||

| another separating | plane: w= (1,0) == 1/2 Separating plane plane: W X+b= 1
(1) (1) -1= 1 WX+b=-1 (1,1)(-1)-1=-1 <(-1,1)-> (0,1) <(1,1)+> <(0,0),-> (20) +> X+Y-1=0 w=(1,1), b=-1 Distance from (1,1) +> to the plane (Wall), b=-1 $\frac{(1,1)\binom{1}{1}-1}{\sqrt{2}} = \frac{1}{\sqrt{2}} = \frac{1$ is : We could have represented X+Y-1=0 as (w=(2,2) b=-2); 2×+24-2=0 Then the Oplane would be WX+6=3. (2,2)(1)-7=2 [] plane would be (2,2) []-2 = -2 W X + 5 = -2

For the second plane w= (1,0), b=-1/2: Check <(1,1),+>: (1,0)(1)-1/2=1/2. Not good, since we want to separate the positive points better, so we scale < w, 6>: (C, 0) (1) - = 1 = That's what we want =) c-1/2=1 C=2. =) We rename the plane to be w=(2,0), b=-1 Now: $+: (2, 0) \binom{1}{1} - |=|$ + : $(2, 0) \begin{pmatrix} z \\ z \end{pmatrix} - 1 = 3$ -: (2,0) (-/)=1=-3 $-: (2, 0) \binom{0}{0} = 1 = -1$ 600d But, now ||w|| = |(2,0)|= 2 Before we had ||w|| = |(1)|| = 2, Better

Available on the web site

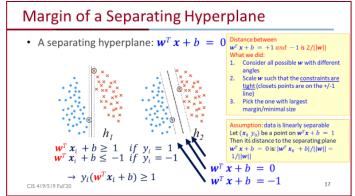
- Remember that all the lectures are available on the website before the class
 - Go over it and be prepared
 - A new set of written notes will accompany most lectures, with some more details, examples and, (when relevant) some code.
- HW 3: Due on 11/16/20
 - You cannot solve all the problems yet.
 - Less time consuming; no programming
- Cheating
 - Several problems in HW1 and HW2

Projects

- CIS 519 students need to do a team project: Read the project descriptions
 - Teams will be of size 2-4
 - We will help grouping if needed
- There will be 3 projects.
 - Natural Language Processing (Text)
 - Computer Vision (Images)
 - Speech (Audio)
- In all cases, we will give you datasets and initial ideas
 - The problem will be multiclass classification problems
 - You will get annotated data only for some of the labels, but will also have to predict other labels
 - O-zero shot learning; few-shot learning; transfer learning
- A detailed note will come out today.
- Timeline:
 - 11/11 Choose a project and team up
 - 11/23 Initial proposal describing what your team plans to do
 - 12/2 Progress report
 - 12/15-20 (TBD) Final paper + short video
- Try to make it interesting!

Hard SVM Optimization

- We have shown that the sought-after weight vector w is the solution of the following optimization problem:
 - SVM Optimization: (***)
 - Minimize: $\frac{1}{2} ||w||^2$
 - Subject to: $\forall (x, y) \in S$: $y w^T x \ge 1$



- This is a quadratic optimization problem in (n + 1) variables, with |S| = m inequality constraints.
- It has a unique solution.

Maximal Margin

$$\min_{\boldsymbol{w},b} \quad \frac{1}{2} \boldsymbol{w}^T \boldsymbol{w}$$

s.t $y_i (\boldsymbol{w}^T \boldsymbol{x}_i + b) \ge 1, \forall (\boldsymbol{x}_i, y_i) \in S$

Support Vector Machines

- The name "Support Vector Machine" stems from the fact that w^{*} is supported by (i.e. is the linear span of) the examples that are exactly at a distance 1/||w^{*}|| from the separating hyperplane. These vectors are therefore called support vectors.
- Theorem: Let w^* be the minimizer of the SVM optimization problem (***) for $S = \{(x_i, y_i)\}$. Let $I = \{i: w^{*T}x_i = 1\}$. Then there exists coefficients $\alpha_i > 0$ such that: $w^* = \sum_{i \in I} \alpha_i y_i x_i$ This representation should ring a bell...

How did we call this representation of w?

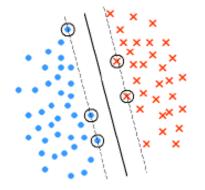


Start the presentation to see live content. For screen share software, share the entire screen. Get help at pollev.com/app

Duality

- This, and other properties of Support Vector Machines are shown by moving to the <u>dual problem</u>.
- Theorem: Let w* be the minimizer of the SVM optimization problem (***) for S = {(x_i, y_i)}. Let I = { i: y_i(w*Tx_i + b) = 1}. Then there exists coefficients α_i > 0 such that:

$$\boldsymbol{w}^* = \sum_{i \in I} \alpha_i \, y_i \, \boldsymbol{x}_i$$



Footnote about the threshold

- Similar to Perceptron, we can augment vectors to handle the bias term $\overline{x} \leftarrow (x, 1); \ \overline{w} \leftarrow (w, b)$ so that $\overline{w}^T \overline{x} = w^T x + b$
- Then consider the following formulation

 $\min_{\overline{\boldsymbol{w}}} \quad \frac{1}{2} \, \overline{\boldsymbol{w}}^T \, \overline{\boldsymbol{w}} \quad \text{ s.t } \quad y_i \, \overline{\boldsymbol{w}}^T \, \overline{\boldsymbol{x}}_i \geq 1, \, \forall (\boldsymbol{x}_i, y_i) \in \mathbb{S}$

• However, this formulation is slightly different from (***), because it is equivalent to

$$\min_{\boldsymbol{w},\boldsymbol{b}} \quad \frac{1}{2} \boldsymbol{w}^T \boldsymbol{w} + \frac{1}{2} \boldsymbol{b}^2 \quad \text{s.t} \quad y_i(\boldsymbol{w}^T \mathbf{x}_i + \boldsymbol{b}) \ge 1, \forall (\boldsymbol{x}_i, y_i) \in S$$

The bias term is included in the regularization. This usually doesn't matter

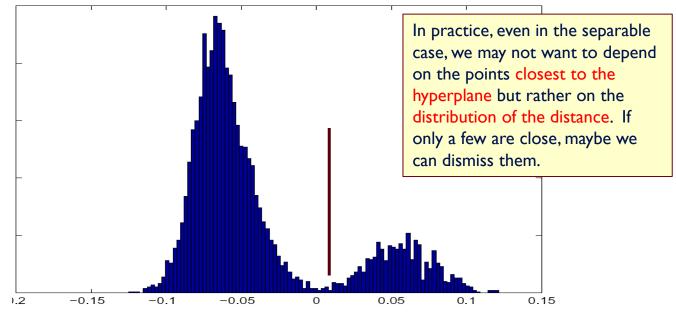
For simplicity, we ignore the bias term

Key Issues

- Computational Issues
 - Training of an SVM used to be is very time consuming solving quadratic program.
 - Modern methods are based on Stochastic Gradient Descent and Coordinate Descent and are much faster.
- Is it really optimal?
 - Is the objective function we are optimizing the "right" one?

Real Data

- 17,000 dimensional context sensitive spelling
- Histogram of distance of points from the hyperplane



Soft SVM

- The hard SVM formulation assumes linearly separable data.
- A natural relaxation:
 - maximize the margin while minimizing the # of examples that violate the margin (separability) constraints.
- However, this leads to non-convex problem that is hard to solve.
- Instead, we relax in a different way, that results in optimizing a surrogate loss function that is convex.

Soft SVM

- Notice that the relaxation of the constraint: $y_i w^T x_i \ge 1$
- Can be done by introducing a slack variable ξ_i (per example) and requiring:

$$y_i \boldsymbol{w}^T \boldsymbol{x}_i \geq 1 - \xi_i ; \xi_i \geq 0$$

• Now, we want to solve:

$$\min_{\boldsymbol{w},\xi_i} \quad \frac{1}{2} \boldsymbol{w}^T \boldsymbol{w} + C \sum_i \xi_i$$

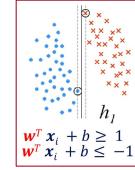
• A large value of C means that we want ξ_i to be small; that is, misclassifications are bad – we focus on a small training error (at the expense of margin).

• A small C results in more training error, but hopefully better true error.

s.t $y_i \mathbf{w}^T \mathbf{x}_i \ge 1 - \xi_i$; $\xi_i \ge 0 \quad \forall i$

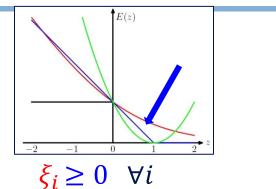
Soft SVM (2)

• Now, we want to solve:



$$\min_{\boldsymbol{w},\xi_i} \quad \frac{1}{2} \boldsymbol{w}^T \boldsymbol{w} + C \sum_i \xi_i$$

s.t
$$\xi_i \ge 1 - y_i \mathbf{w}^T x_i$$



In optimum, $\xi_i = \max(0, 1 - y_i \mathbf{w}^T \mathbf{x}_i)$

• Which can be written as:

$$\min_{\boldsymbol{w}} \quad \frac{1}{2} \boldsymbol{w}^T \boldsymbol{w} + C \sum_i \max(0, 1 - y_i \boldsymbol{w}^T \boldsymbol{x}_i).$$

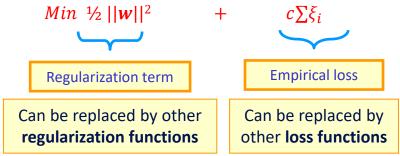
• What is the interpretation of this?

SVM Objective Function

• The problem we solved is:

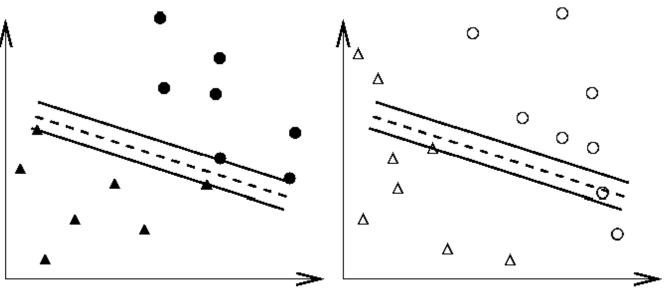
 $Min \frac{1}{2} ||\mathbf{w}||^2 + c \sum \xi_i$

- Where $\xi_i > 0$ is called a slack variable, and is defined by:
 - $\xi_i = \max(0, 1 y_i \boldsymbol{w}^T \boldsymbol{x}_i)$
 - Equivalently, we can say that: $y_i w^T x_i \ge 1 \xi_i; \xi_i \ge 0$
- And this can be written as:



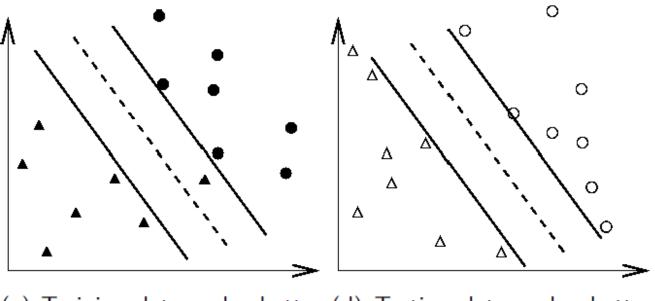
- General Form of a learning algorithm:
 - Minimize empirical loss, and Regularize (to avoid over fitting)
 - Theoretically motivated improvement over the original algorithm we've seen at the beginning of the semester.

Balance between regularization and empirical loss



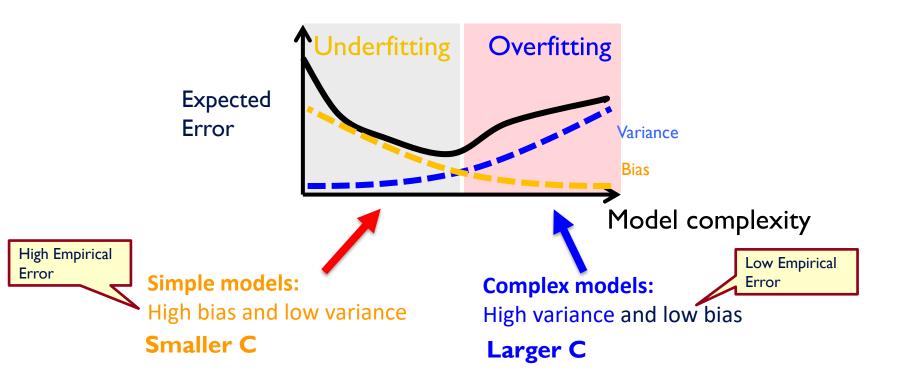
(a) Training data and an over- (b) Testing data and an overfitting classifier fitting classifier

Balance between regularization and empirical loss



(c) Training data and a better (d) Testing data and a better classifier classifier

Underfitting and Overfitting

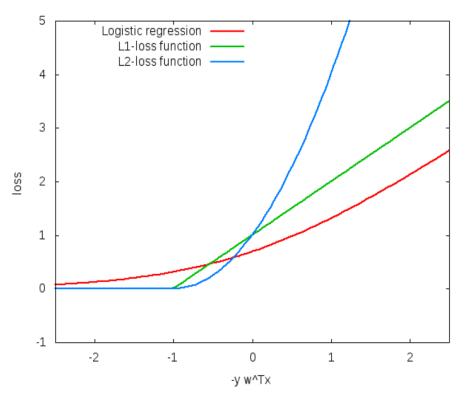


- L1-loss SVM $\min_{\boldsymbol{w}} \frac{1}{2} \boldsymbol{w}^T \boldsymbol{w} + C \sum_{i=1}^{l} \max(0, 1 - y_i \boldsymbol{w}^T \boldsymbol{x}_i)$
- L2-loss SVM

$$\min_{w} \frac{1}{2} w^{T} w + C \sum_{i=1}^{l} \max(0, 1 - y_{i} w^{T} x_{i})^{2}$$

What Do We Optimize(2)?

- We get an unconstrained problem.
 We can use the (stochastic) gradient descent algorithm!
- Many other methods
 - Iterative scaling; non-linear conjugate gradient; quasi-Newton methods; truncated Newton methods; trustregion newton method.
 - All methods are iterative methods, that generate a sequence w_k that converges to the optimal solution of the optimization problem above.
- Currently: Limited memory BFGS is very popular



Optimization: How to Solve

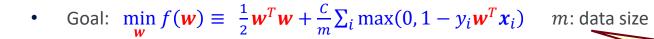
1. Earlier methods used Quadratic Programming. Very slow.

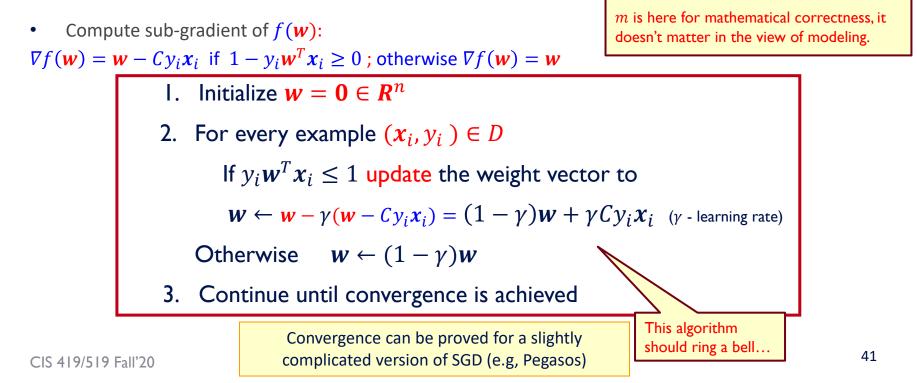
2. The soft SVM problem is an unconstrained optimization problems. It is possible to use the gradient descent algorithm.

- Many options within this category:
 - Iterative scaling; non-linear conjugate gradient; quasi-Newton methods; truncated Newton methods; trust-region newton method.
 - All methods are iterative methods, that generate a sequence w_k that converges to the optimal solution of the optimization problem above.
 - Currently: Limited memory BFGS is very popular
- 3. 3rd generation algorithms are based on Stochastic Gradient Decent
 - The runtime does not depend on n = #(examples); advantage when n is very large.
 - Stopping criteria is a problem: method tends to be too aggressive at the beginning and reaches a moderate accuracy quite fast, but it's convergence becomes slow if we are interested in more accurate solutions.

4. Dual Coordinated Descent (& Stochastic Version)

SGD for SVM



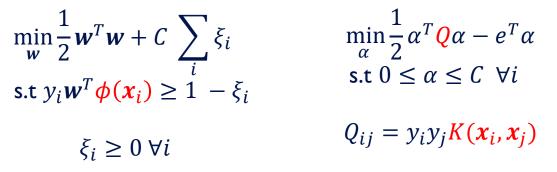


Nonlinear SVM

- We can map data to a high dimensional space: $x \to \phi(x)$ (DEMO)
- Then use Kernel trick: $K(x_i, x_j) = \phi(x_i)^T \phi(x_j)$ (DEMO2)

Primal

Dual



Theorem: Let w^* be the minimizer of the primal problem, α^* be the minimizer of the dual problem. Then $w^* = \sum_i \alpha^* y_i x_i$

Nonlinear SVM

- Tradeoff between training time and accuracy
- Complex model vs. simple model

	Linear (LIBLINEAR)			RBF (LIBSVM)			
Data set	C	Time (s)	Accuracy	C	σ	Time (s)	Accuracy
a9a	32	5.4	84.98	8	0.03125	98.9	85.03
real-sim	1	0.3	97.51	8	0.5	973.7	97.90
ijcnn1	32	1.6	92.21	32	2	26.9	98.69
MNIST38	0.03125	0.1	96.82	2	0.03125	37.6	99.70
covtype	0.0625	1.4	76.35	32	32	54,968.1	96.08
webspam	32	25.5	93.15	8	32	$15,\!571.1$	99.20

From:

http://www.csie.ntu.edu.tw/~cjlin/papers/lowpoly_journal.pdf