

Support Vector Machines (SVM)

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



Midterm Exams

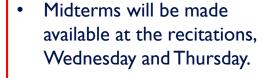
Questions?

Overall (142):

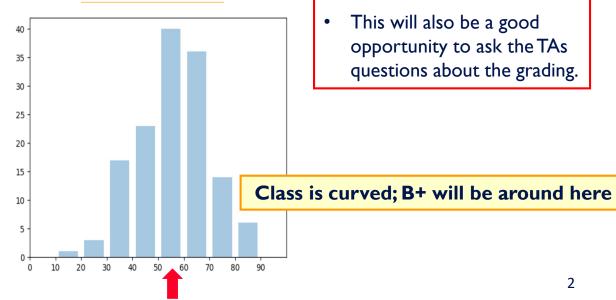
– Mean: 55.36

Std Dev: 14.9

Max: 98.5, Min: 1



Solutions will be available tomorrow.



Projects

- Please start working!
- Come to my office hours at least once in the next 3 weeks to discuss the project.
- HW2 Grades are out too.

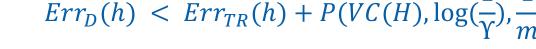
	PDF (40)	Code (60)	Total (100)	EC (10)
Mean	35.96	54.79	88.51	0.74
Stdev	6.8	12.75	23.12	2.47
Max	40	60	100	10
Min	1.5	0	0	0
# submissions	143	139	-	-

- HW3 is out.
 - You can only do part of it now. Hopefully can do it all by Wednesday.

COLT approach to explaining Learning

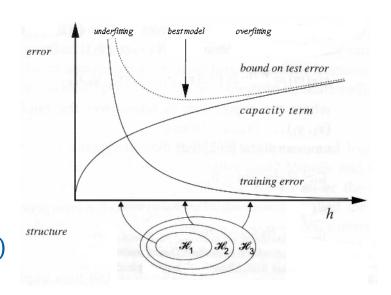
- No Distributional Assumption
- Training Distribution is the same as the Test Distribution
- Generalization bounds depend on this view and affects model selection.

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



This is also called the

"Structural Risk Minimization" principle.



COLT approach to explaining Learning

- No Distributional Assumption
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$$Err_D(h) < Err_{TR}(h) + P(VC(H), \log(1/\Upsilon), 1/m)$$

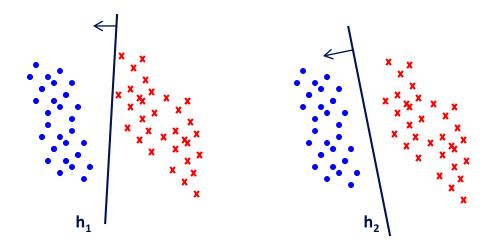
- As presented, the VC dimension is a combinatorial parameter that is associated with a class of functions.
- We know that the class of linear functions has a lower VC dimension than the class of quadratic functions.
- But, this notion can be refined to depend on a given data set, and this way directly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



VC and Linear Classification

Recall the VC based generalization bound:

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

Here we get the same bound for both classifiers:

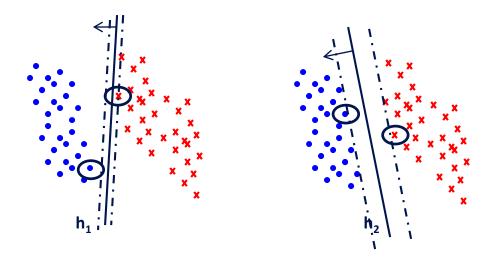
$$Err_{TR}(h_1) = Err_{TR}(h_2) = 0$$

 $h_1, h_2 \in H_{lin(2)}, VC(H_{lin(2)}) = 3$

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

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

• The margin of a set of points $\{x_1, ... x_m\}$ 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_{Υ} is the space of all linear classifiers in \mathbb{R}^n that separate the training data with margin at least Υ , then:

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

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

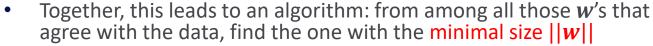
$$Err(h) \le err_{TR}(h) + \left\{ \frac{o\left(\frac{R^2}{\gamma^2}\right) + \log\left(\frac{4}{\delta}\right)}{m} \right\}^{1/2}$$

Towards Max Margin Classifiers

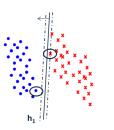
- First observation: When we consider the class H_{Υ} of linear hypotheses that separate a given data set with a margin Υ , we see that
 - − Large Margin Υ → Small VC dimension of H_{Υ}

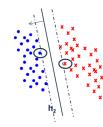
But, how can we do it algorithmically?

- 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



- But, if w separates the data, so does w/7....
- We need to better understand the relations between w and the margin

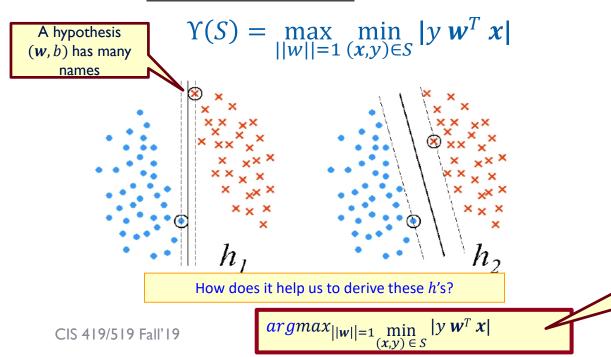




Maximal Margin

The distance between a point
$$x$$
 and the hyperplane defined by $(w; b)$ is:
$$|w^T x + b|/||w||$$

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



- 1. For a given w: Find the closest point.
- 2. Then, find the point that gives the maximal margin value across all w's (of size 1).

Note: the selection of the point is in the min and therefore the max does not change if we scale **w**, so it's okay to only deal with normalized **w**'s.

Interpretation 1: among all w's, choose the one that maximizes the margin.

Recap: Margin and VC dimension

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.

 We'll show this
- 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:

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

- How to find this w*?
- Claim: Define \mathbf{w}_0 to be the solution of the optimization problem

-
$$\mathbf{w}_0 = argmin\{||\mathbf{w}||^2 : \forall (x,y) \in S, y \mathbf{w}^T x \ge 1\}.$$

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

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

The next slide will show that the two interpretations are equivalent

From Margin to ||w||(2)

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

```
\mathbf{w}_0 = argmin\{||\mathbf{w}||^2 : \forall (x,y) \in S, y \mathbf{w}^T x \geq 1\}
Then:
- w_0/||w_0|| = argmax_{||w||=1} \min_{(x,y) \in S} y w^T x
```

That is, the normalization of \mathbf{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 $w' = w^*$. Def. of

Note first that $\frac{w^*}{\gamma(\varsigma)}$ satisfies the constraints in (**);

therefore:
$$||w_0|| \le ||w^*/\Upsilon(S)|| = 1/\Upsilon(S)$$
. Consequently: Def. of w' Def. of w_0

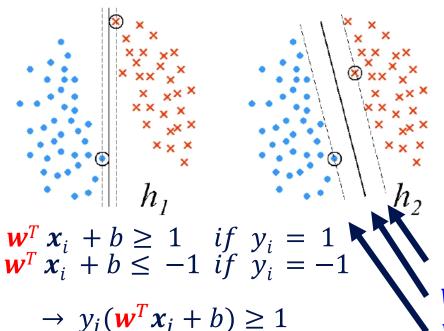
$$\forall (x, y) \in S \ y \ w'^T \ x = \frac{1}{||w_0||} y w_0^T \ x \ge 1/||w_0|| \ge \Upsilon(S)$$

But since ||w'|| = 1 this implies that w' corresponds to the largest margin, that is

$$w' = w^*$$

Margin of a Separating Hyperplane

• A separating hyperplane: $\mathbf{w}^T \mathbf{x} + \mathbf{b} = \mathbf{0}$



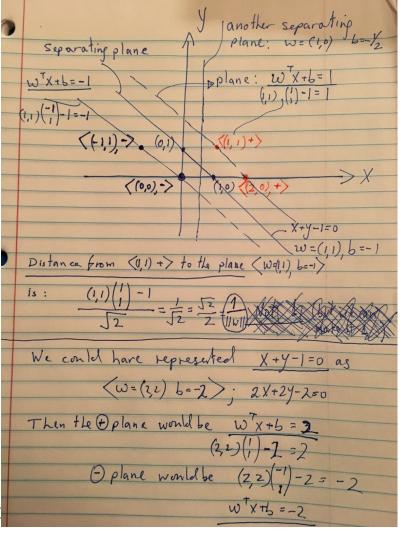
Distance between

 $w^T x + b = +1 \text{ and } -1 \text{ is } 2/||w||$ What we did:

- Consider all possible w with different angles
- 2. Scale **w** such that the constraints are tight
- 3. Pick the one with largest margin/minimal size

Assumption: data is linearly separable Let (x_0, y_0) be a point on $\mathbf{w}^T \mathbf{x} + b = 1$ Then its distance to the separating plane $\mathbf{w}^T \mathbf{x} + b = 0$ is: $|\mathbf{w}^T \mathbf{x}_0| + b|/||\mathbf{w}|| = 1/||\mathbf{w}||$

$$\mathbf{w}^T \mathbf{x} + b = 0$$
$$\mathbf{w}^T \mathbf{x} + b = -1$$



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>: (Co) (1) - = 1 = That's what we want =) (-1/2) (=2. => We rename the plane to be W=(2,0), 5=-1 Now: +: (2,0)(1)-1=1 +: (2,0)(2)-1=3 -: (2,0) -/ = 1=-3 -: (2,0)(0) = 1 = -1600d Brt now ||w|| = 1/(2,0) 1 = 2 Before we had ||w|| = |(1,1)| = 12, Befor

Hard SVM Optimization

 We have shown that the sought after weight vector w is the solution of the following optimization problem:

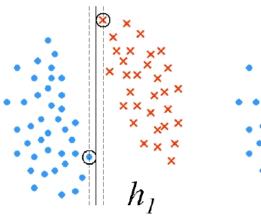
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SVM Optimization: (***)

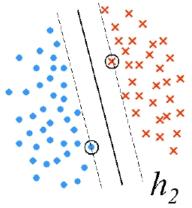
- Minimize: \frac{1}{2} ||w||^2

- 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





The margin of a linear separator $\mathbf{w}^T \mathbf{x} + b = 0$ is $\frac{2}{||\mathbf{w}||}$

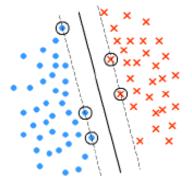
$$\max \frac{2}{||w||} = \min ||w||$$
$$= \min \frac{1}{2} w^T w$$

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

Support Vector Machines

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

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



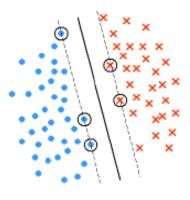
This representation should ring a bell...

Duality

- This, and other properties of Support Vector Machines are shown by moving to the <u>dual problem</u>.
- Theorem: Let \mathbf{w}^* be the minimizer of the SVM optimization problem (***) for $S = \{(\mathbf{x}_i, \mathbf{y}_i)\}$. Let $I = \{i: y_i(\mathbf{w}^{*T}\mathbf{x}_i + b) = 1\}$.

Then there exists coefficients $\alpha_i > 0$

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



such that:

Footnote about the threshold

• Similar to Perceptron, we can augment vectors to handle the bias term

$$\overline{x} \leftarrow (x, 1); \ \overline{w} \leftarrow (w, b) \ \text{ so that } \overline{w}^T \overline{x} = w^T x + b$$

• Then consider the following formulation

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

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

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

The bias term is included in the regularization.

This usually doesn't matter

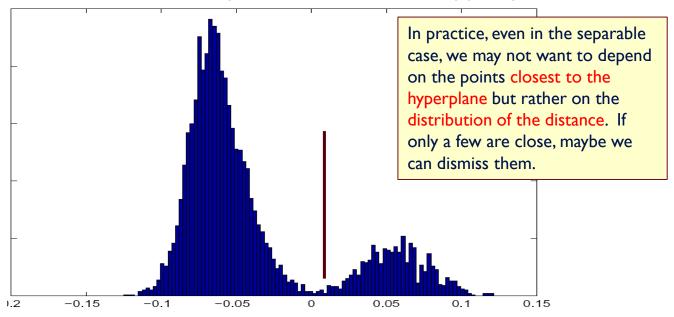
For simplicity, we ignore the bias term

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



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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.

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Soft SVM

Notice that the relaxation of the constraint:

$$y_i \mathbf{w}^T \mathbf{x}_i \ge 1$$

• Can be done by introducing a slack variable ξ_i (per example) and requiring:

$$y_i \mathbf{w}^T \mathbf{x}_i \ge 1 - \xi_i$$
; $\xi_i \ge 0$

Now, we want to solve:

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

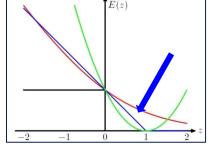
A large value of C means that misclassifications are bad – we focus on a small training error (at the expense of margin). A small C results in more training error, but hopefully better true error.

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

Soft SVM (2)

Now, we want to solve:

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



s.t
$$\xi_i \ge 1 - y_i \mathbf{w}^T x_i \ \xi_i \ge 0 \ \forall i$$

Which can be written as:

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

$$\min_{\mathbf{w}} \ \frac{1}{2} \mathbf{w}^T \mathbf{w} + C \sum_{i} \max(0, 1 - y_i \mathbf{w}^T \mathbf{x}_i).$$

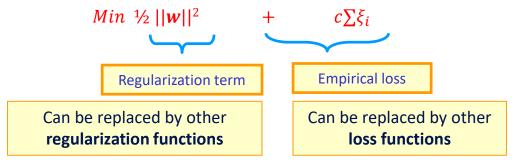
What is the interpretation of this?

SVM Objective Function

The problem we solved is:

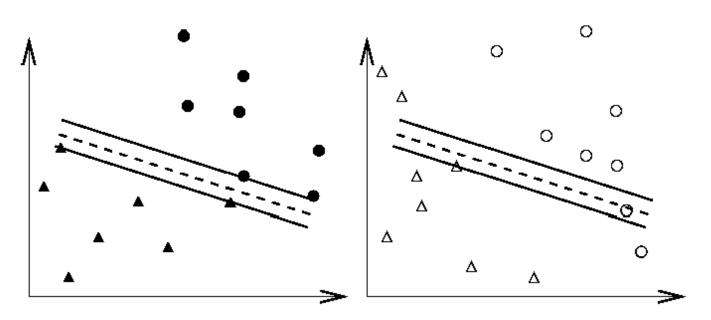
$$Min \frac{1}{2} ||\mathbf{w}||^2 + c \sum \xi_i$$

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

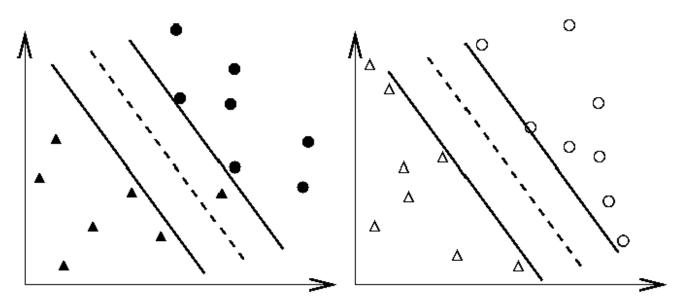
Balance between regularization and empirical loss



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

fitting classifier

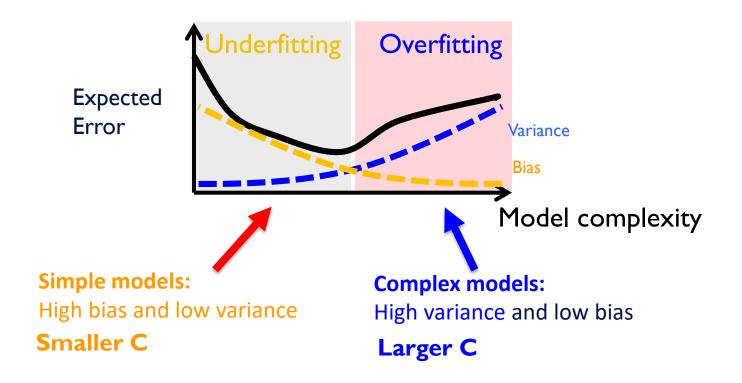
Balance between regularization and empirical loss



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



Underfitting and Overfitting



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What Do We Optimize?

Logistic Regression

$$\min_{\mathbf{w}} \frac{1}{2} \mathbf{w}^{T} \mathbf{w} + C \sum_{i=1}^{l} \log(1 + e^{-y_{i}(\mathbf{w}^{T} x_{i})})$$

L1-loss SVM

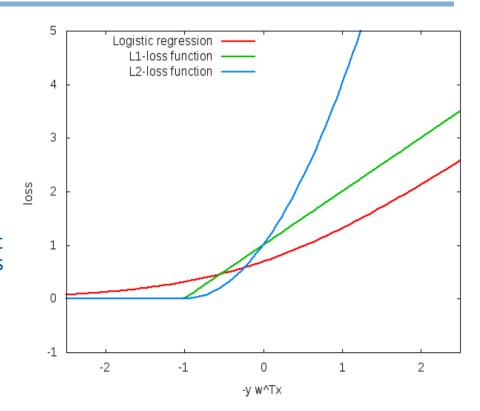
$$\min_{\mathbf{w}} \frac{1}{2} \mathbf{w}^T \mathbf{w} + C \sum_{i=1}^{l} \max(0,1 - y_i \mathbf{w}^T \mathbf{x}_i)$$

L2-loss SVM

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

What Do We Optimize(2)?

- We get an unconstrained problem.
 We can use the gradient descent algorithm! However, it is quite slow.
- 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 \mathbf{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 \mathbf{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)

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SGD for SVM

- Goal: $\min_{\mathbf{w}} f(\mathbf{w}) \equiv \frac{1}{2} \mathbf{w}^T \mathbf{w} + \frac{c}{m} \sum_{i} \max(0, 1 y_i \mathbf{w}^T \mathbf{x}_i)$ m: data size
- Compute sub-gradient of f(w):

$$\nabla f(\mathbf{w}) = \mathbf{w} - Cy_i \mathbf{x}_i$$
 if $1 - y_i \mathbf{w}^T \mathbf{x}_i \ge 0$; otherwise $\nabla f(\mathbf{w}) = \mathbf{w}$

m is here for mathematical correctness, it doesn't matter in the view of modeling.

- I. Initialize $\mathbf{w} = \mathbf{0} \in \mathbb{R}^n$
- 2. For every example $(x_i, y_i) \in D$

If $y_i \mathbf{w}^T \mathbf{x}_i \leq 1$ update the weight vector to

$$\mathbf{w} \leftarrow (1 - \gamma)\mathbf{w} + \gamma C y_i \mathbf{x}_i$$
 (γ - learning rate)

Otherwise $w \leftarrow (1 - \gamma)w$

3. Continue until convergence is achieved

Convergence can be proved for a slightly complicated version of SGD (e.g, Pegasos)

This algorithm should ring a bell...

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

$$\min_{\mathbf{w}} \frac{1}{2} \mathbf{w}^{T} \mathbf{w} + C \sum_{i} \xi_{i} \qquad \min_{\alpha} \frac{1}{2} \alpha^{T} \mathbf{Q} \alpha - e^{T} \alpha
\text{s.t } y_{i} \mathbf{w}^{T} \phi(\mathbf{x}_{i}) \ge 1 - \xi_{i} \qquad \text{s.t } 0 \le \alpha \le C \ \forall i
\xi_{i} \ge 0 \ \forall i \qquad Q_{ij} = y_{i} y_{j} K(\mathbf{x}_{i}, \mathbf{x}_{j})$$

Theorem: Let w^* be the minimizer of the primal problem, α^* be the minimizer of the dual problem.

Then
$$\mathbf{w}^* = \sum_i \alpha^* y_i \mathbf{x}_i$$

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