Support Vector Machines

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CSG220
Spring 2007

Adapted from the Andrew Moore tutorial of the same name

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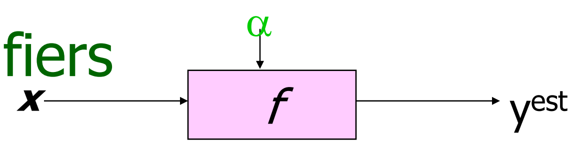
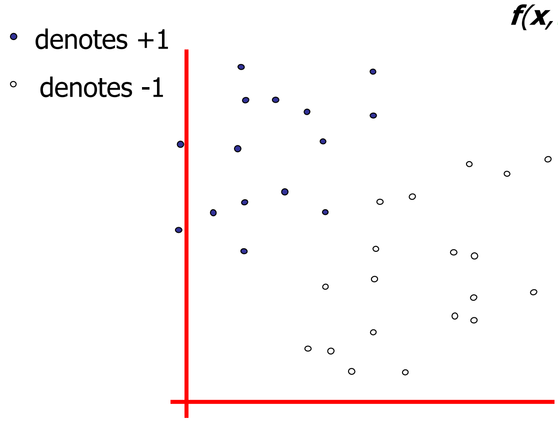
Linear Classifiers

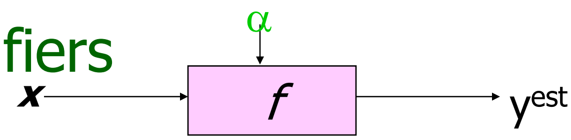


$f(\mathbf{x},\mathbf{w},b) = sgn(\mathbf{w}\cdot\mathbf{x} + b)$



How would you classify this data?

Linear Classifiers



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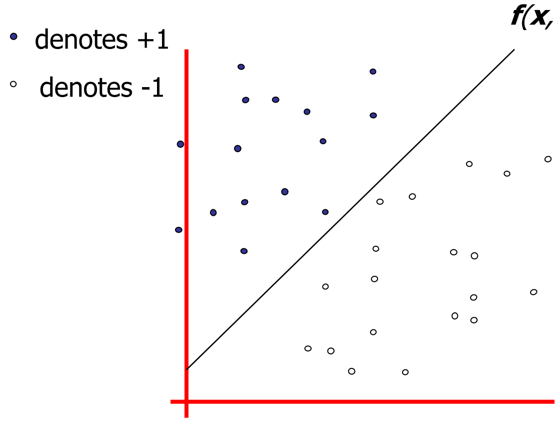

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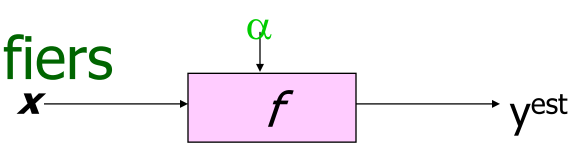

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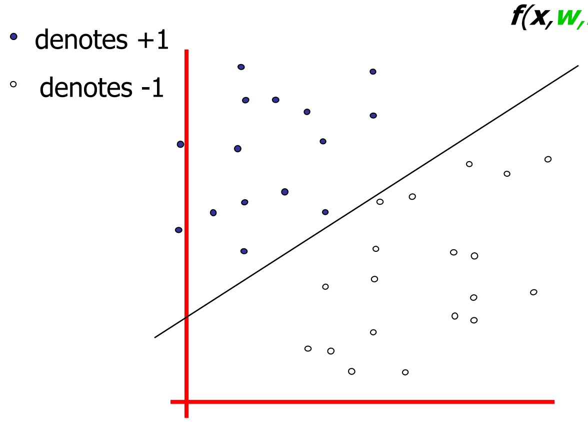

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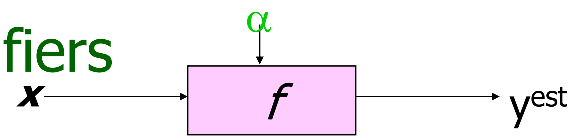
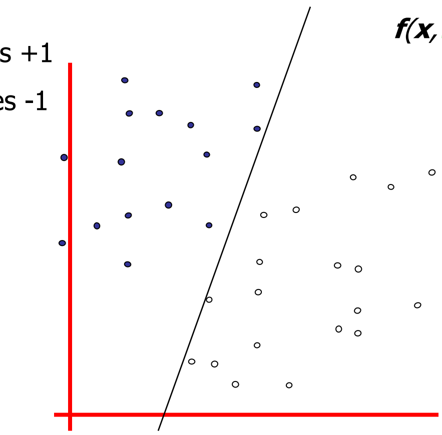


$f(\mathbf{x},\mathbf{w},b) = sgn(\mathbf{w} \cdot \mathbf{x} + b)$

- denotes +1
- denotes -1



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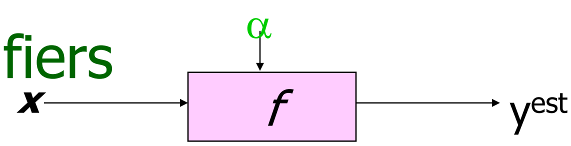

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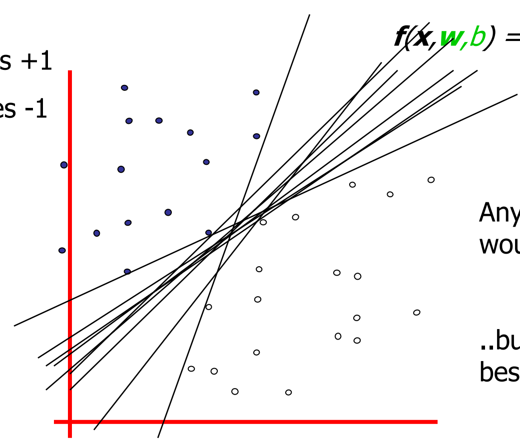
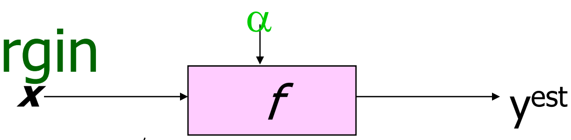


Any of these would be fine..

..but which is best?

Classifier Margin



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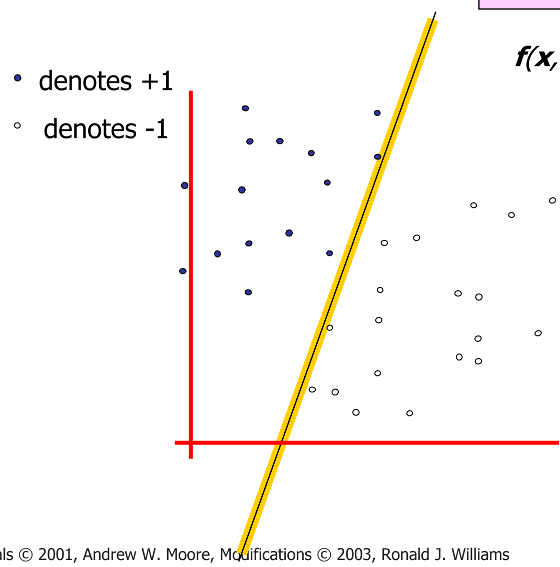
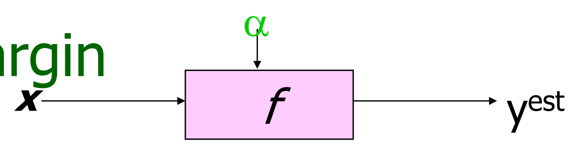


Define the margin of a linear classifier as the perpendicular distance from the decision boundary to the nearest datapoint.

Maximum Margin



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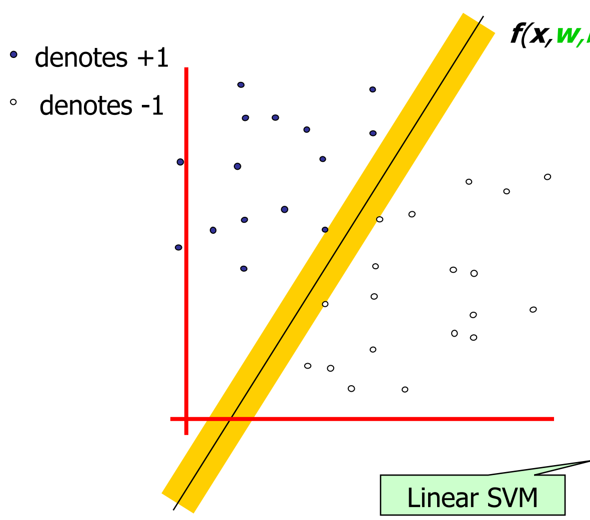
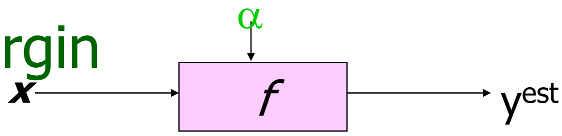


The maximum margin linear classifier is the linear classifier with the, um, maximum margin.

This is the simplest kind of SVM (Called an LSVM)

Maximum Margin



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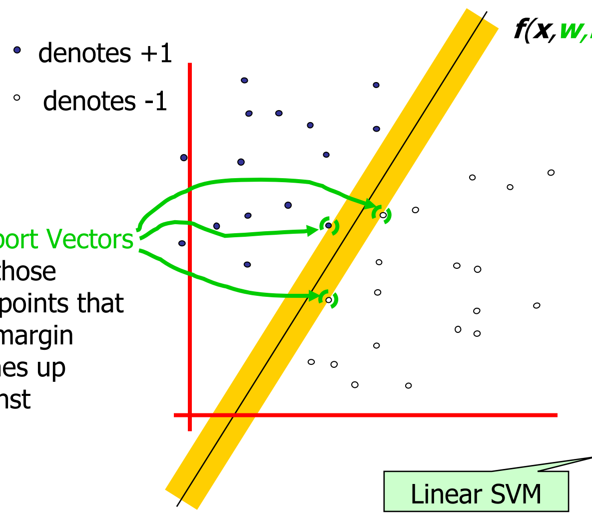

Support Vectors are those datapoints that the margin pushes up against

The maximum margin linear classifier is the linear classifier with the, um, maximum margin.

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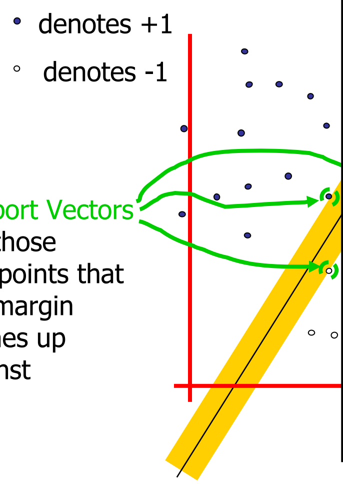
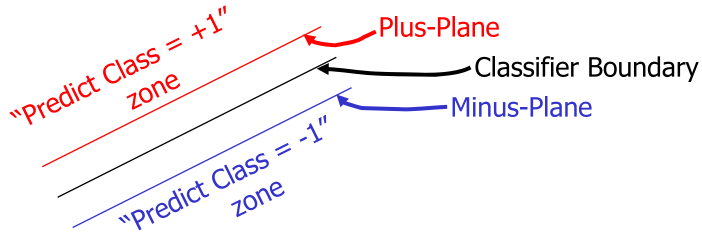
Why Maximum Margin?



Support Vectors are those datapoints that the margin pushes up against

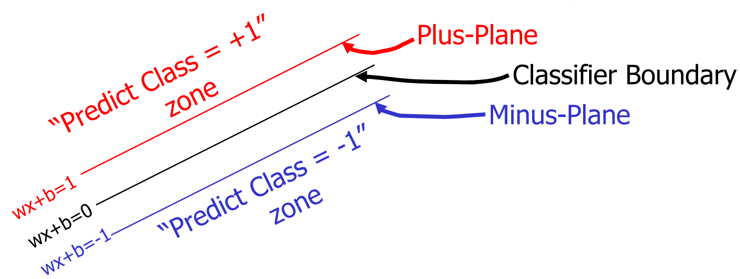
1. Intuitively this feels safest.
2. If we've made a small error in the location of the boundary (it's been jolted in its perpendicular direction) this gives us least chance of causing a misclassification.
3. LOOCV is easy since the model is immune to removal of any non-support-vector datapoints.
4. There's some theory (using VC dimension) that is related to (but not the same as) the proposition that this is a good thing.
5. Empirically it works very very well.

Specifying a line and margin



- How do we represent this mathematically?
- …in *m* input dimensions?

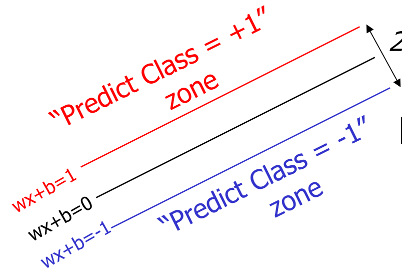
Specifying a line and margin



- Plus-plane = $\{\, \mathbf{x} : \mathbf{w} \cdot \mathbf{x} + b = +1 \,\}$
- Minus-plane = $\{\, \mathbf{x} : \mathbf{w} \cdot \mathbf{x} + b = -1 \,\}$

Classify as..	+1	if	$\mathbf{w} \cdot \mathbf{x} + b >= 1$
	-1	if	$\mathbf{w} \cdot \mathbf{x} + b <= -1$
	Universe explodes	if	$-1 < \mathbf{w} \cdot \mathbf{x} + b < 1$

Computing the margin width



2M where *M* = Margin Width

How do we compute *M* in terms of ***w*** and *b*?

- Plus-plane = $\{ \mathbf{x} : \mathbf{w} \cdot \mathbf{x} + b = +1 \}$
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Claim: The vector **w** is perpendicular to the Plus Plane. Why?

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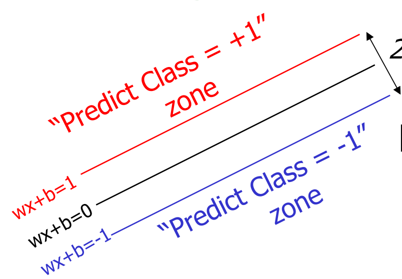

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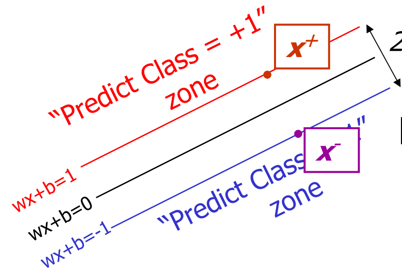
Claim: The vector **w** is perpendicular to the Plus Plane. Why?

Let **u** and **v** be two vectors on the Plus Plane. What is $\mathbf{w} \cdot (\mathbf{u} - \mathbf{v})$?

And so of course the vector **w** is also perpendicular to the Minus Plane

Computing the margin width



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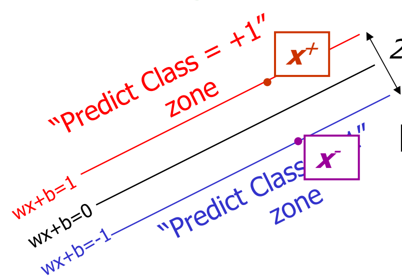
- The vector **w** is perpendicular to the Plus Plane
- Let $\mathbf{x}^-$ be any point on the minus plane
- Let $\mathbf{x}^+$ be the closest plus-plane-point to $\mathbf{x}^-$.

Any location in R^m: not necessarily a datapoint

 Support Vector Machines: Slide 15

Computing the margin width



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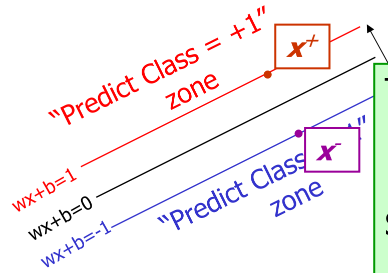
- Claim: $\mathbf{x}^+ = \mathbf{x}^- + \lambda\, \mathbf{w}$ for some value of λ. Why?

 Support Vector Machines: Slide 16

Computing the margin width



2M where *M* = Margin Width

The line from $\boldsymbol{x}^-$ to $\boldsymbol{x}^+$ is perpendicular to the planes.

So to get from $\boldsymbol{x}^-$ to $\boldsymbol{x}^+$ travel some distance in direction $\boldsymbol{w}$.

- Plus-plane = $\{ \boldsymbol{x} : \boldsymbol{w} \cdot \boldsymbol{x} + b$
- Minus-plane = $\{ \boldsymbol{x} : \boldsymbol{w} \cdot \boldsymbol{x} + b = -1 \}$
- The vector **w** is perpendicular to the Plus Plane
- Let $\boldsymbol{x}^-$ be any point on the minus plane
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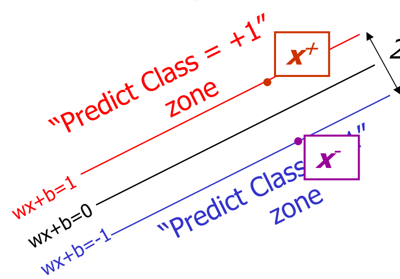
Computing the margin width



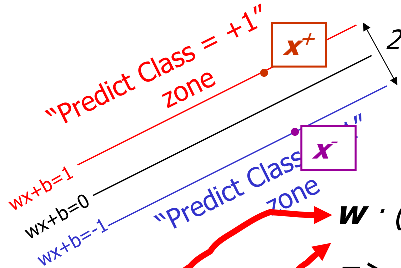
2M where *M* = Margin Width

What we know:

- $\boldsymbol{w} \cdot \boldsymbol{x}^+ + b = +1$
- $\boldsymbol{w} \cdot \boldsymbol{x}^- + b = -1$
- $\boldsymbol{x}^+ = \boldsymbol{x}^- + \lambda \boldsymbol{w}$
- $||\boldsymbol{x}^+ - \boldsymbol{x}^- || = 2M$

It's now easy to get *M* in terms of $\boldsymbol{w}$ and *b*

Computing the margin width



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- $|\boldsymbol{x}^+ - \boldsymbol{x}^-| = 2M$

It's now easy to get *M* in terms of ***w*** and *b*

$\boldsymbol{w} \cdot (\boldsymbol{x}^- + \lambda \boldsymbol{w}) + b = 1$

=>

$\boldsymbol{w} \cdot \boldsymbol{x}^- + b + \lambda \boldsymbol{w} \cdot \boldsymbol{w} = 1$

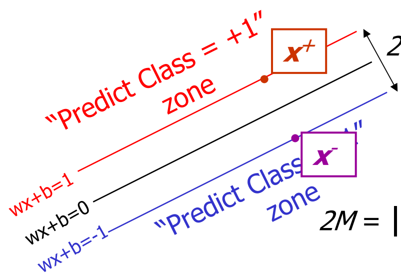
=>

$-1 + \lambda \boldsymbol{w} \cdot \boldsymbol{w} = 1$

=>

$$\lambda = \frac{2}{\|\mathbf{w}\|^2}$$

Computing the margin width



$2M = \frac{2}{\|\mathbf{w}\|}$ so $M = \frac{1}{\|\mathbf{w}\|}$

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- $\boldsymbol{w} . \boldsymbol{x}^+ + b = +1$
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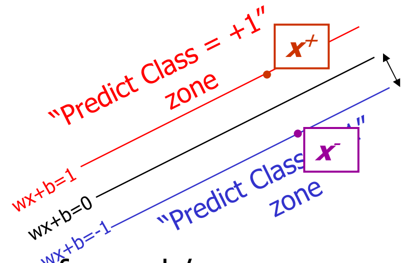
- $\boldsymbol{x}^+ = \boldsymbol{x}^- + \lambda \boldsymbol{w}$
- $|\boldsymbol{x}^+ - \boldsymbol{x}^-| = 2M$
- $\lambda = \frac{2}{\|\mathbf{w}\|^2}$

$$2M = |\boldsymbol{x}^+ - \boldsymbol{x}^-| = |\lambda \boldsymbol{w}|$$

$$= \lambda \|\mathbf{w}\| = \frac{2}{\|\mathbf{w}\|^2}\|\mathbf{w}\| = \frac{2}{\|\mathbf{w}\|}$$

$$\text{Therefore } M = \frac{1}{\|\mathbf{w}\|}$$

Learning the Maximum Margin Classifier



M = Margin Width = $\frac{1}{\|\mathbf{w}\|}$

Given a guess of ***w*** and *b* we can

- Compute whether all data points in the correct half-planes
- Compute the width of the margin

So now we just need to write a program to search the space of **w**'s and *b*'s to find the widest margin that matches all the datapoints. *How?*

Gradient descent? Simulated Annealing? Matrix Inversion? EM? Newton's Method?

Learning via Quadratic Programming

- QP is a well-studied class of optimization algorithms to maximize a quadratic function of some real-valued variables subject to linear constraints.

Quadratic Programming

Find $\arg\max_{\mathbf{u}} \quad c + \mathbf{d}^T\mathbf{u} + \dfrac{\mathbf{u}^T R\mathbf{u}}{2}$ ⟵ Quadratic criterion

Subject to

$$\left.\begin{aligned} a_{11}u_1 + a_{12}u_2 + \ldots + a_{1m}u_m &\le b_1 \\ a_{21}u_1 + a_{22}u_2 + \ldots + a_{2m}u_m &\le b_2 \\ &\vdots \\ a_{n1}u_1 + a_{n2}u_2 + \ldots + a_{nm}u_m &\le b_n \end{aligned}\right\} \text{n additional linear inequality constraints}$$

And subject to

$$\left.\begin{aligned} a_{(n+1)1}u_1 + a_{(n+1)2}u_2 + \ldots + a_{(n+1)m}u_m &= b_{(n+1)} \\ a_{(n+2)1}u_1 + a_{(n+2)2}u_2 + \ldots + a_{(n+2)m}u_m &= b_{(n+2)} \\ &\vdots \\ a_{(n+e)1}u_1 + a_{(n+e)2}u_2 + \ldots + a_{(n+e)m}u_m &= b_{(n+e)} \end{aligned}\right\} \text{e additional linear equality constraints}$$

Quadratic Programming

Find $\arg\max_{\mathbf{u}} \quad c + \mathbf{d}^T\mathbf{u} + \dfrac{\mathbf{u}^T R\mathbf{u}}{2}$ ⟵ Quadratic criterion

Subject to

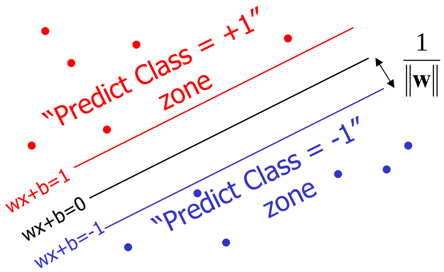
There exist algorithms for finding such constrained quadratic optima much more efficiently and reliably than gradient ascent. Really good news: There are no non-global optima in QP problems.

(But these algorithms are very fiddly…you probably don't want to write one yourself)

And subject to

e additional linear equality constraints

Learning the Maximum Margin Classifier



Given guess of ***w*** , *b* we can

- Compute whether all data points are in the correct half-planes
- Compute the margin width

Assume *R* datapoints $(\mathbf{x}_k, y_k)$ where $y_k = \pm 1$

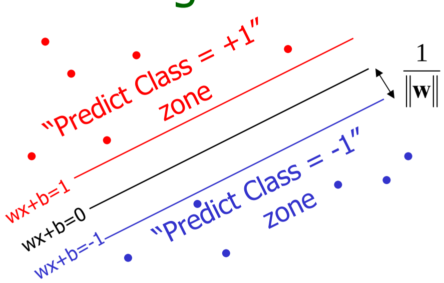
What should our quadratic optimization criterion be?

How many constraints will we have?

What should they be?

 Support Vector Machines: Slide 25

Learning the Maximum Margin Classifier



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What should our quadratic optimization criterion be?

Minimize $\|\mathbf{w}\|^2 = \mathbf{w} \cdot \mathbf{w}$

How many constraints will we have? *R*

What should they be?

$\mathbf{w} \cdot \mathbf{x}_k + b \geq 1 \text{ if } y_k = 1$

$\mathbf{w} \cdot \mathbf{x}_k + b \leq -1 \text{ if } y_k = -1$

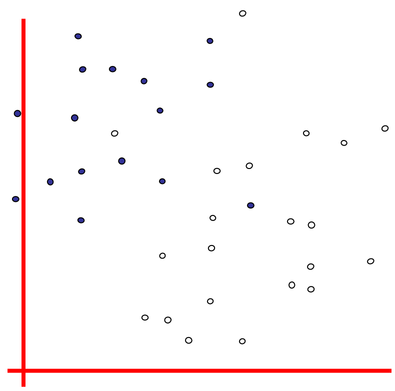
 Support Vector Machines: Slide 26

Uh-oh!

This is going to be a problem!

What should we do?

- denotes +1
- denotes -1



Uh-oh!

This is going to be a problem!

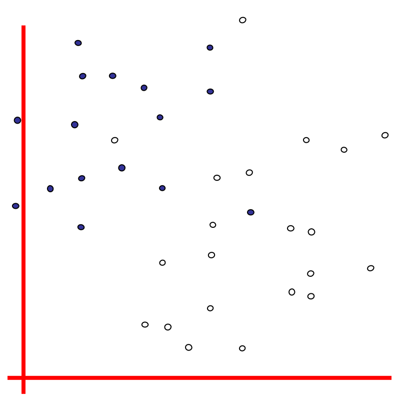
What should we do?

Idea 1:

Find minimum $\mathbf{w'w}$, while minimizing number of training set errors.

Problemette: Two things to minimize makes for an ill-defined optimization

- denotes +1
- denotes -1



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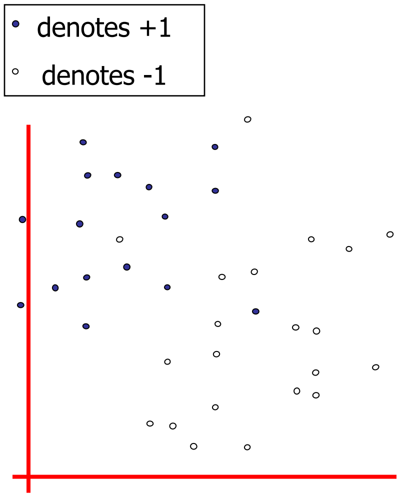


This is going to be a problem!

What should we do?

Idea 1.1:

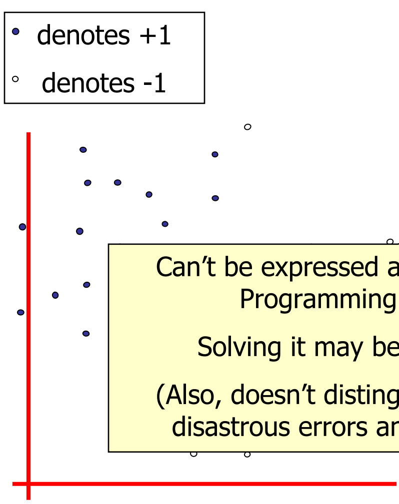
Minimize

$\boldsymbol{w \cdot w} + C\,(\#\text{train errors})$

Tradeoff parameter

There's a serious practical problem that's about to make us reject this approach. Can you guess what it is?

Uh-oh!



This is going to be a problem!

What should we do?

Idea 1.1:

Minimize

$\boldsymbol{w \cdot w} + C\,(\#\text{train errors})$

Tradeoff parameter

Can't be expressed as a Quadratic Programming problem.

Solving it may be too slow.

(Also, doesn't distinguish between disastrous errors and near misses)

So… any other ideas?

Uh-oh!

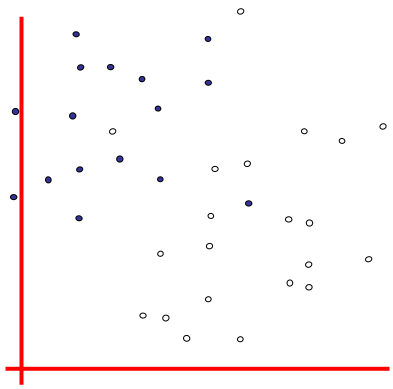
This is going to be a problem!

What should we do?

Idea 2.0:

Minimize
w·w *+ C (distance of error points to their correct place)*

• denotes +1
◦ denotes -1



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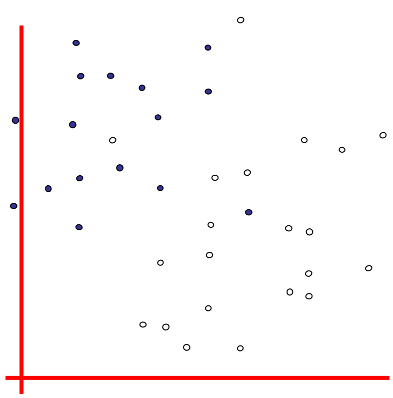
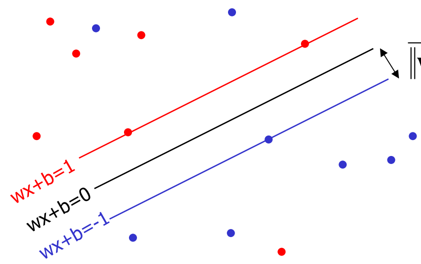


Called soft-margin SVM

Learning Maximum Margin with Noise



$\frac{1}{\|\mathbf{w}\|}$

Given guess of $\boldsymbol{w}$, b we can

- Compute sum of distances of points to their correct zones
- Compute the margin width

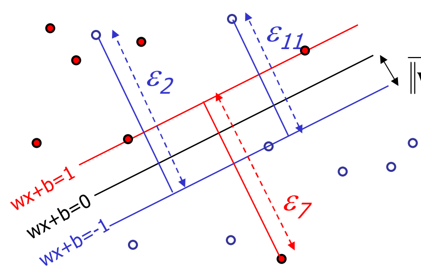
Assume R datapoints $(\boldsymbol{x}_k, y_k)$ where $y_k = \pm 1$

What should our quadratic optimization criterion be?

How many constraints will we have?

What should they be?

Learning Maximum Margin with Noise



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Assume R datapoints $(\boldsymbol{x}_k, y_k)$ where $y_k = \pm 1$

What should our quadratic optimization criterion be?

Minimize $\frac{1}{2}\mathbf{w}\cdot\mathbf{w} + C\sum_{k=1}^{R}\varepsilon_k$

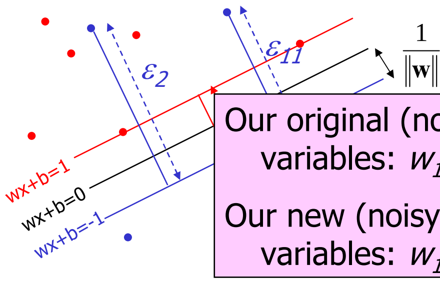
How many constraints will we have? R

What should they be?

$\boldsymbol{w} \cdot \boldsymbol{x}_k + b \geq 1-\varepsilon_k$ if $y_k = 1$

$\boldsymbol{w} \cdot \boldsymbol{x}_k + b \leq -1+\varepsilon_k$ if $y_k = -1$

Learning Maximum Margin with Noise



m = # input dimensions

Given gu… we can

- Compute sum of distances …

Our original (noiseless data) QP had $m+1$ variables: $w_1, w_2, \ldots w_m$, and b.

Our new (noisy data) QP has $m+1+R$ variables: $w_1, w_2, \ldots w_m, b, \varepsilon_k, \varepsilon_1, \ldots \varepsilon_R$

R= # records

What should our quadratic optimization criterion be?

Minimize $\frac{1}{2}\mathbf{w}\cdot\mathbf{w} + C\sum_{k=1}^{R}\varepsilon_k$

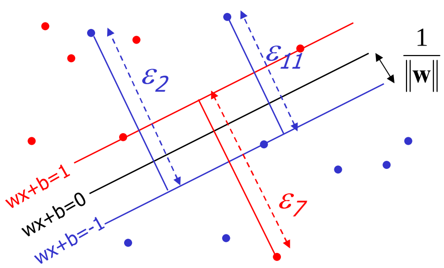
How many constraints will we have? *R*

What should they be?

$\mathbf{w} \cdot \mathbf{x}_k + b \geq 1-\varepsilon_k$ if $y_k = 1$

$\mathbf{w} \cdot \mathbf{x}_k + b \leq -1+\varepsilon_k$ if $y_k = -1$

Learning Maximum Margin with Noise



Given guess of $\mathbf{w}$, b we can

- Compute sum of distances of points to their correct zones
- Compute the margin width

Assume *R* datapoints $(\mathbf{x}_k, y_k)$ where $y_k = \pm 1$

What should our quadratic optimization criterion be?

Minimize $\frac{1}{2}\mathbf{w}\cdot\mathbf{w} + C\sum_{k=1}^{R}\varepsilon_k$

How many constraints will we have? *R*

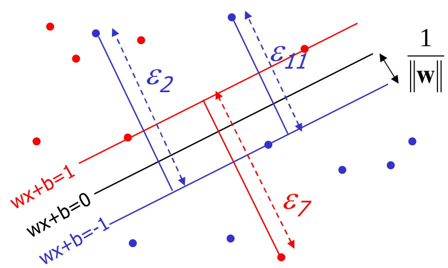
What should they be?

$\mathbf{w} \cdot \mathbf{x}_k + b \geq 1-\varepsilon_k$ if $y_k = 1$

$\mathbf{w} \cdot \mathbf{x}_k + b \leq -1+\varepsilon_k$ if $y_k = -1$

There's a bug in this QP. Can you spot it?

Learning Maximum Margin with Noise



Given guess of ***w*** , *b* we can

- Compute sum of distances of points to their correct zones
- Compute the margin width

Assume *R* datapoints $(\mathbf{x}_k, y_k)$ where $y_k = \pm 1$

What should our quadratic optimization criterion be?

Minimize $$\frac{1}{2}\mathbf{w}\cdot\mathbf{w} + C\sum_{k=1}^{R}\varepsilon_k$$

How many constraints will we have? *2R*

What should they be?

$\mathbf{w} \cdot \mathbf{x}_k + b \geq 1-\varepsilon_k$ if $y_k = 1$

$\mathbf{w} \cdot \mathbf{x}_k + b \leq -1+\varepsilon_k$ if $y_k = -1$

$\varepsilon_k \geq 0$ for all k

An Equivalent QP

Maximize $$\sum_{k=1}^{R}\alpha_k + \sum_{k=1}^{R}\sum_{l=1}^{R}\alpha_k\alpha_l Q_{kl} \quad \text{where} \quad Q_{kl} = y_k y_l(\mathbf{x}_k \cdot \mathbf{x}_l)$$

Subject to these constraints: $$0 \leq \alpha_k \leq C \quad \forall k \qquad \sum_{k=1}^{R}\alpha_k y_k = 0$$

Then define:

$$\mathbf{w} = \sum_{k=1}^{R}\alpha_k y_k \mathbf{x}_k$$

$$b = y_i - \mathbf{x}_i \cdot \mathbf{w}$$

where $0 < \alpha_i < C$

Then classify with:

$f(\mathbf{x},\mathbf{w},b) = sgn(\mathbf{w} \cdot \mathbf{x} + b)$

An Equivalent QP

Maximize $\sum_{k=1}^{R} \alpha_k + \sum_{k=1}^{R} \sum_{l=1}^{R} \alpha_k \alpha_l Q_{kl}$ where $Q_{kl} = y_k y_l (\mathbf{x}_k \cdot \mathbf{x}_l)$

Subject to these constraints: $0 \le \alpha_k \le C \quad \forall k \qquad \sum_{k=1}^{R} \alpha_k y_k = 0$

Then define:

$$\mathbf{w} = \sum_{k=1}^{R} \alpha_k y_k \mathbf{x}_k$$

$$b = y_i - \mathbf{x}_i \cdot \mathbf{w}$$

where $0 < \alpha_i < C$

Datapoints with $\alpha_k > 0$ will be the support vectors

..so this sum only needs to be over the support vectors.

$f(\mathbf{x},\mathbf{w},b) = sgn(\mathbf{w} \cdot \mathbf{x} + b)$

An Equivalent QP

Why did I tell you about this equivalent QP? (Dual QP)

- It's a formulation that QP packages can optimize more quickly
- And especially because of further jaw-dropping developments you're about to learn.

But first ...

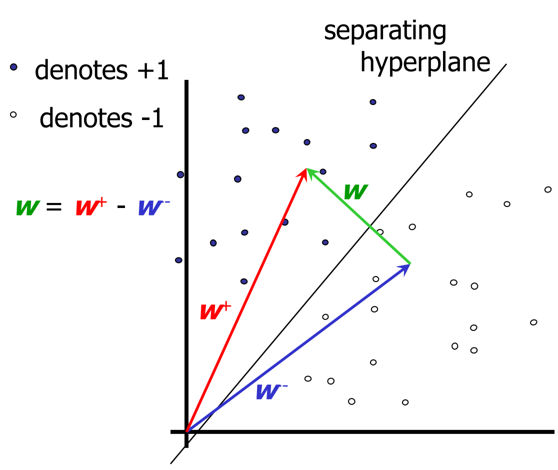
- Let's compare the two QP formulations
  - Original solves for *m+1+R* numbers
    - weights ***w*** and bias *b*
    - slack variables ε_k (one per data point)
  - Dual solves for *R+1* numbers
    - bias b and one α_k per data point
- Consider

m = dimension of ***w***

$$\mathbf{w} = \sum_{k=1}^{R} \alpha_k y_k \mathbf{x}_k$$

  - Expresses ***w*** in terms of a new basis consisting of the instance vectors $\boldsymbol{x}_k$
  - What's this all about?

Using the instances as a basis



$$I^+ = \{i \mid y_i = +1\}$$

$$I^- = \{i \mid y_i = -1\}$$

$$\mathbf{w}^+ = \sum_{i \varepsilon I^+} \alpha_i \mathbf{x}_i \,, \quad \alpha_i \geq 0$$

$$\mathbf{w}^- = \sum_{i \varepsilon I^-} \alpha_i \mathbf{x}_i \,, \quad \alpha_i \geq 0$$

$$\begin{aligned} \mathbf{w} &= \mathbf{w}^+ - \mathbf{w}^- \\ &= \sum_{i \varepsilon I^+} \alpha_i \mathbf{x}_i - \sum_{i \varepsilon I^-} \alpha_i \mathbf{x}_i \\ &= \sum_i \alpha_i y_i \mathbf{x}_i \end{aligned}$$

Obviously, coefficients not unique in general

Perceptron algorithm: dual version

- Even our old familiar perceptron algorithm can be expressed using the instances as a basis
- Let's review the original version ...

Perceptron algorithm revisited

$\mathbf{w} \leftarrow \mathbf{0}$

$b \leftarrow 0$

Repeat

For $i = 1$ to R

If $y_i(\mathbf{w} \cdot \mathbf{x}_i + b) \leq 0$

$\mathbf{w} \leftarrow \mathbf{w} + \eta y_i \mathbf{x}_i$

$b \leftarrow b + \eta y_i$

Until no errors

A concise way to test for incorrect classification

Classify arbitrary $\boldsymbol{x}$ according to $\mathrm{sgn}(\mathbf{w} \cdot \mathbf{x} + b)$

Perceptron algorithm: dual version

- Notice that ***w*** can be written as

$$\eta y_{i_1}\mathbf{x}_{i_1} + \eta y_{i_2}\mathbf{x}_{i_2} + \cdots + \eta y_{i_m}\mathbf{x}_{i_m}$$

where i_1, i_2, ..., i_m are the indices of the succession of training data for which errors occur.

- Written more concisely,

$$\mathbf{w} = \sum_{i=i_1}^{i_m} \eta y_i \mathbf{x}_i$$

- Similarly,

$$b = \sum_{i=i_1}^{i_m} \eta y_i$$

Perceptron algorithm: dual form

- Note that the same *i* may occur multiple times among the indices i_1, i_2, ..., i_m representing the succession of training data causing weight changes (i.e., one training pattern may lead to multiple weight changes as the algorithm proceeds).
- Regrouping the sums according to the indexing of the training data, we get

$$\mathbf{w} = \sum_{i=1}^{R} \alpha_i \eta y_i \mathbf{x}_i \quad \text{and} \quad b = \sum_{i=1}^{R} \alpha_i \eta y_i$$

where α_i is a nonnegative integer counting the number of times the training pattern $(\mathbf{x}_i, y_i)$ contributed to a weight correction

Perceptron algorithm: dual form

Classification of an arbitrary ***x*** is then given by

$$\operatorname{sgn}(\mathbf{w}\cdot\mathbf{x}+b) = \operatorname{sgn}\left(\left(\sum_{i=1}^{R}\alpha_i\eta y_i\mathbf{x}_i\right)\cdot\mathbf{x}+\sum_{i=1}^{R}\alpha_i\eta y_i\right)$$

$$= \operatorname{sgn}\left(\sum_{i=1}^{R}\alpha_i\eta y_i\mathbf{x}_i\cdot\mathbf{x}+\sum_{i=1}^{R}\alpha_i\eta y_i\right)$$

$$= \operatorname{sgn}\left(\sum_{i=1}^{R}\alpha_i y_i\mathbf{x}_i\cdot\mathbf{x}+\sum_{i=1}^{R}\alpha_i y_i\right)$$

Learning the dual form directly

- To learn the quantities $\alpha_1, \alpha_2, \ldots, \alpha_R$ and b directly, replace the body of the inner loop by

$$\alpha_i \leftarrow \alpha_i + 1$$
$$b \leftarrow b + y_i$$

- If the data are not linearly separable, the α_i values grow without bound for misclassified points
- Each α_i is a measure of how much the instance $\boldsymbol{x}_i$ contributes to the classification
- Thus the familiar perceptron algorithm provides one example of how linear classifiers can be expressed in terms of the data vectors themselves

Classification using the dual form

- Given any $\alpha_1, \alpha_2, \ldots, \alpha_R$ and *b* (however obtained), the classification of arbitrary ***x*** is given by

$$\mathrm{sgn}\left(\sum_{i=1}^{R} \alpha_i y_i \mathbf{x}_i \cdot \mathbf{x} + b \right)$$

- Has the flavor of an instance-based method
    - classify by comparing (in this case computing the dot product of) the new instance with all the training instances
    - but training instances with $\alpha_i = 0$ (e.g., non-support vectors in SVMs) can be ignored

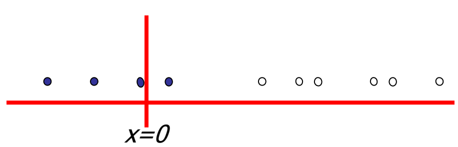
- Now back to SVMs ...

Nonlinear SVMs: The "kernel trick"

- So far we've covered Linear SVMs only
  - Hard-margin (requires linear separability)
  - Soft-margin (tolerates nonlinear separability)
- What if we want to form nonlinear separations?
- Simple solution
  - Map data into a higher-dimensional feature space
  - Find linear separations in this new space
- Magically, all the bad things that would ordinarily happen with this approach don't   That's why it's a trick!
- Let's start with some simple examples ...

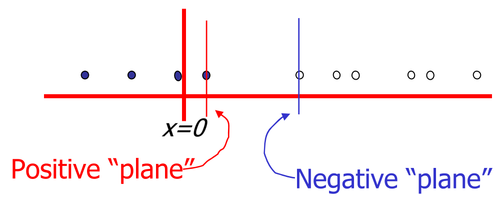
Suppose we're in 1-dimension

What would SVMs do with this data?

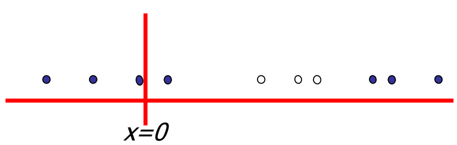


Suppose we're in 1-dimension

Not a big surprise



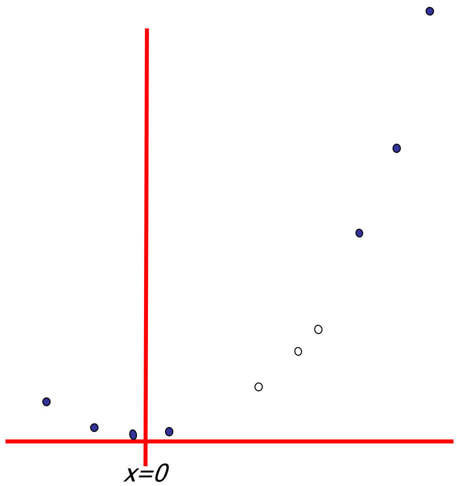
Harder 1-dimensional dataset



That's wiped the smirk off SVM's face.

What can be done about this?

Harder 1-dimensional dataset

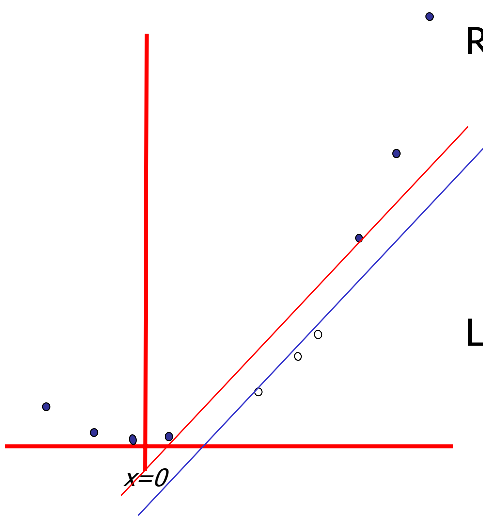


Remember how permitting non-linear basis functions made linear regression so much nicer?

Let's permit them here too

$$\mathbf{z}_k = (x_k, x_k^2)$$

Harder 1-dimensional dataset



Remember how permitting non-linear basis functions made linear regression so much nicer?

Let's permit them here too

$$\mathbf{z}_k = (x_k, x_k^2)$$

Common SVM basis functions

$\boldsymbol{z}_k$ = (polynomial terms of $\boldsymbol{x}_k$ of degree 0 to q)

$\boldsymbol{z}_k$ = (radial basis functions of $\boldsymbol{x}_k$)

$$\mathbf{z}_k[j] = \varphi_j(\mathbf{x}_k) = \text{KernelFn}\left(\frac{|\mathbf{x}_k - \mathbf{c}_j|}{\text{KW}}\right)$$

$\boldsymbol{z}_k$ = (sigmoid functions of $\boldsymbol{x}_k$)

This is sensible.

Is that the end of the story?

No…here's where the trick comes in!

Quadratic Basis Functions

$$\Phi(\mathbf{x}) = \begin{pmatrix} 1 \\ \sqrt{2}x_1 \\ \sqrt{2}x_2 \\ : \\ \sqrt{2}x_m \\ x_1^2 \\ x_2^2 \\ : \\ x_m^2 \\ \sqrt{2}x_1x_2 \\ \sqrt{2}x_1x_3 \\ : \\ \sqrt{2}x_1x_m \\ \sqrt{2}x_2x_3 \\ : \\ \sqrt{2}x_1x_m \\ : \\ \sqrt{2}x_{m-1}x_m \end{pmatrix}$$

Constant Term

Linear Terms

Pure Quadratic Terms

Quadratic Cross-Terms

Number of terms (assuming m input dimensions) = (m+2)-choose-2

= (m+2)(m+1)/2

= (as near as makes no difference) $m^2/2$

You may be wondering what those $\sqrt{2}$'s are doing.

- You should be happy that they do no harm
- You'll find out why they're there soon.

QP with basis functions

Maximize $\sum_{k=1}^{R} \alpha_k + \sum_{k=1}^{R} \sum_{l=1}^{R} \alpha_k \alpha_l Q_{kl}$ where $Q_{kl} = y_k y_l (\mathbf{\Phi}(\mathbf{x}_k) \cdot \mathbf{\Phi}(\mathbf{x}_l))$

Subject to these constraints: $0 \le \alpha_k \le C \quad \forall k$ $\quad \sum_{k=1}^{R} \alpha_k y_k = 0$

Then define:

$$\mathbf{w} = \sum_k \alpha_k y_k \mathbf{\Phi}(\mathbf{x}_k)$$

$$b = y_i - \mathbf{\Phi}(\mathbf{x}_i) \cdot \mathbf{w}$$

$$\text{where } 0 < \alpha_i < C$$

Then classify with:

f(x,w,b) *= sgn(**w** · Φ(**x**) + b)*

All we've done here is to replace every vector ***x*** in the instance space in the earlier description with its corresponding feature vector ***Φ(x)***

QP with basis functions

Maximize $\sum_{k=1}^{R} \alpha_k + \sum_{k=1}^{R} \sum_{l=1}^{R} \alpha_k \alpha_l Q_{kl}$ where $Q_{kl} = y_k y_l (\mathbf{\Phi}(\mathbf{x}_k) \cdot \mathbf{\Phi}(\mathbf{x}_l))$

We must do $R^2/2$ dot products to get this matrix ready.

Each dot product requires $m^2/2$ additions and mutiplications

The whole thing costs $R^2 m^2 /4$. Yeeks!

...or does it?

Subject to these constraints: $0 \le \alpha_k \le$

Then define:

$$\mathbf{w} = \sum_k \alpha_k y_k \mathbf{\Phi}(\mathbf{x}_k)$$

$$b = y_i - \mathbf{\Phi}(\mathbf{x}_i) \cdot \mathbf{w}$$

$$\text{where } 0 < \alpha_i < C$$

f(x,w,b) *= sgn(**w** · Φ(**x**) + b)*

All we've done here is to replace every vector ***x*** in the instance space in the earlier description with its corresponding feature vector ***Φ(x)***

Quadratic Dot Products

$$
\Phi(\mathbf{a}) \bullet \Phi(\mathbf{b}) =
\begin{pmatrix}
1 \\ \sqrt{2}a_1 \\ \sqrt{2}a_2 \\ : \\ \sqrt{2}a_m \\ a_1^2 \\ a_2^2 \\ : \\ a_m^2 \\ \sqrt{2}a_1a_2 \\ \sqrt{2}a_1a_3 \\ : \\ \sqrt{2}a_1a_m \\ \sqrt{2}a_2a_3 \\ : \\ \sqrt{2}a_1a_m \\ : \\ \sqrt{2}a_{m-1}a_m
\end{pmatrix}
\bullet
\begin{pmatrix}
1 \\ \sqrt{2}b_1 \\ \sqrt{2}b_2 \\ : \\ \sqrt{2}b_m \\ b_1^2 \\ b_2^2 \\ : \\ b_m^2 \\ \sqrt{2}b_1b_2 \\ \sqrt{2}b_1b_3 \\ : \\ \sqrt{2}b_1b_m \\ \sqrt{2}b_2b_3 \\ : \\ \sqrt{2}b_1b_m \\ : \\ \sqrt{2}b_{m-1}b_m
\end{pmatrix}
$$

$$1$$

$$+$$

$$\sum_{i=1}^{m} 2a_ib_i$$

$$+$$

$$\sum_{i=1}^{m} a_i^2b_i^2$$

$$+$$

$$\sum_{i=1}^{m}\sum_{j=i+1}^{m} 2a_ia_jb_ib_j$$

Quadratic Dot Products

$$\Phi(\mathbf{a}) \bullet \Phi(\mathbf{b}) =$$

$$1 + 2\sum_{i=1}^{m} a_ib_i + \sum_{i=1}^{m} a_i^2b_i^2 + \sum_{i=1}^{m}\sum_{j=i+1}^{m} 2a_ia_jb_ib_j$$

Just out of casual, innocent, interest, let's look at another function of ***a*** and ***b***:

$$(\mathbf{a}\cdot\mathbf{b}+1)^2$$

$$= (\mathbf{a}\cdot\mathbf{b})^2 + 2\mathbf{a}\cdot\mathbf{b} + 1$$

$$= \left(\sum_{i=1}^{m} a_ib_i\right)^2 + 2\sum_{i=1}^{m} a_ib_i + 1$$

$$= \sum_{i=1}^{m}\sum_{j=1}^{m} a_ib_ia_jb_j + 2\sum_{i=1}^{m} a_ib_i + 1$$

$$= \sum_{i=1}^{m} (a_ib_i)^2 + 2\sum_{i=1}^{m}\sum_{j=i+1}^{m} a_ib_ia_jb_j + 2\sum_{i=1}^{m} a_ib_i + 1$$

Quadratic Dot Products

$$\Phi(\mathbf{a}) \bullet \Phi(\mathbf{b}) =$$
$$1 + 2\sum_{i=1}^{m} a_i b_i + \sum_{i=1}^{m} a_i^2 b_i^2 + \sum_{i=1}^{m} \sum_{j=i+1}^{m} 2 a_i a_j b_i b_j$$

Just out of casual, innocent, interest, let's look at another function of ***a*** and ***b***:

$$(\mathbf{a} \cdot \mathbf{b} + 1)^2$$
$$= (\mathbf{a} \cdot \mathbf{b})^2 + 2\mathbf{a} \cdot \mathbf{b} + 1$$
$$= \left(\sum_{i=1}^{m} a_i b_i \right)^2 + 2\sum_{i=1}^{m} a_i b_i + 1$$
$$= \sum_{i=1}^{m} \sum_{j=1}^{m} a_i b_i a_j b_j + 2\sum_{i=1}^{m} a_i b_i + 1$$
$$= \sum_{i=1}^{m} (a_i b_i)^2 + 2\sum_{i=1}^{m} \sum_{j=i+1}^{m} a_i b_i a_j b_j + 2\sum_{i=1}^{m} a_i b_i + 1$$

They're the same!

And this is only O(m) to compute!

QP with basis functions

Maximize $\sum_{k=1}^{R} \alpha_k + \sum_{k=1}^{R} \sum_{l=1}^{R} \alpha_k \alpha_l Q_{kl}$ where $Q_{kl} = y_k y_l (\Phi(\mathbf{x}_k) \cdot \Phi(\mathbf{x}_l))$

We must do $R^2/2$ dot products to get this matrix ready.

Each dot product now only requires *m* additions and multiplications

Subject to these constraints: $0 \leq \alpha_k \leq$

Then define:

$$\mathbf{w} = \sum_{k} \alpha_k y_k \Phi(\mathbf{x}_k)$$

$$b = y_i - \Phi(\mathbf{x}_i) \cdot \mathbf{w}$$
$$\text{where } 0 < \alpha_i < C$$

Then classify with:

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Higher Order Polynomials

Poly-nomial	$\Phi(x)$	Cost to build Q_{kl} matrix traditionally	Cost if 100 inputs	$\Phi(a) \cdot \Phi(b)$	Cost to build Q_{kl} matrix sneakily	Cost if 100 inputs
Quadratic	All $m^2/2$ terms up to degree 2	$m^2 R^2 /4$	2,500 R^2	$(\mathbf{a} \cdot \mathbf{b}+1)^2$	$m R^2 / 2$	50 R^2
Cubic	All $m^3/6$ terms up to degree 3	$m^3 R^2 /12$	83,000 R^2	$(\mathbf{a} \cdot \mathbf{b}+1)^3$	$m R^2 / 2$	50 R^2
Quartic	All $m^4/24$ terms up to degree 4	$m^4 R^2 /48$	1,960,000 R^2	$(\mathbf{a} \cdot \mathbf{b}+1)^4$	$m R^2 / 2$	50 R^2

QP with basis functions

We must do $R^2/2$ dot products to get this matrix ready.

In 100-d, each dot product now needs 103 operations instead of 75 million

But there are still worrying things lurking away. *What are they?*

$$Q_{kl} = y_k y_l (\mathbf{\Phi}(\mathbf{x}_k) \cdot \mathbf{\Phi}(\mathbf{x}_l))$$

constraints:

$$\forall k \qquad \sum_{k=1}^{R} \alpha_k y_k = 0$$

Then define:

$$\mathbf{w} = \sum_k \alpha_k y_k \mathbf{\Phi}(\mathbf{x}_k)$$

$$b = y_i - \mathbf{\Phi}(\mathbf{x}_i) \cdot \mathbf{w}$$

$$\text{where } \; 0 < \alpha_i < C$$

Then classify with:

$f(\mathbf{x},\mathbf{w},b) = sgn(\mathbf{w} \cdot \mathbf{\Phi}(\mathbf{x}) + b)$

QP with basis functions

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$$Q_{kl} = y_k y_l (\mathbf{\Phi}(\mathbf{x}_k) \cdot \mathbf{\Phi}(\mathbf{x}_l))$$

constraints:

$$\forall k \qquad \sum_{k}^{R} \alpha_k y_k = 0$$

- The fear of overfitting with this enormous number of terms
- The evaluation phase (doing a set of predictions on a test set) will be very expensive *(why?)*

Then define:

$$\mathbf{w} = \sum_k \alpha_k y_k \mathbf{\Phi}(\mathbf{x}_k)$$

$$b = y_i - \mathbf{\Phi}(\mathbf{x}_i) \cdot \mathbf{w}$$

$$\text{where } 0 < \alpha_i < C$$

Then classify with:

***f*(*x*, *w*, *b*) = *sgn*(*w* · Φ(*x*) + *b*)**

QP with basis functions

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But there are still worrying things lurking away. *What are they?*

$$Q_{kl} = y_k y_l (\mathbf{\Phi}(\mathbf{x}_k) \cdot \mathbf{\Phi}(\mathbf{x}_l))$$

The use of Maximum Margin magically makes this not a problem

constraints:

$$\forall k \qquad \sum \alpha_k y_k = 0$$

- The fear of overfitting with this enormous number of terms
- The evaluation phase (doing a set of predictions on a test set) will be very expensive *(why?)*

Because each ***w*** · Φ(***x***) (see below) needs 75 million operations. *What can be done?*

Then define:

$$\mathbf{w} = \sum_k \alpha_k y_k \mathbf{\Phi}(\mathbf{x}_k)$$

$$b = y_i - \mathbf{\Phi}(\mathbf{x}_i) \cdot \mathbf{w}$$

$$\text{where } 0 < \alpha_i < C$$

Then classify with:

***f*(*x*, *w*, *b*) = *sgn*(*w* · Φ(*x*) + *b*)**

QP with Quintic basis functions

We must do $R^2/2$ dot products to get this matrix ready.

In 100-d, each dot product now needs 103 operations instead of 75 million

But there are still worrying things lurking away. What are they?

$$Q_{kl} = y_k y_l(\mathbf{\Phi}(\mathbf{x}_k).\mathbf{\Phi}(\mathbf{x}_l))$$

The use of Maximum Margin magically makes this not a problem

constraints: $\forall k$ $\quad \sum_k \alpha_k y_k = 0$

•The fear of overfitting with this enormous number of terms

•The evaluation phase (doing a set of predictions on a test set) will be very expensive (why?)

Then define:

$$\mathbf{w} = \sum_k \alpha_k y_k \mathbf{\Phi}(\mathbf{x}_k)$$

Because each $\mathbf{w}\cdot\Phi(\mathbf{x})$ (see below) needs 75 million operations. What can be done?

$$\mathbf{w}\cdot\mathbf{\Phi}(\mathbf{x}) = \sum_{k \text{ s.t. } \alpha_k > 0} \alpha_k y_k \mathbf{\Phi}(\mathbf{x}_k)\cdot\mathbf{\Phi}(\mathbf{x})$$
$$= \sum_{k \text{ s.t. } \alpha_k > 0} \alpha_k y_k (\mathbf{x}_k \cdot \mathbf{x} + 1)^5$$

Only *Sm* operations (*S* = # support vectors)

Then classify with:

***f*(*x*,*w*,*b*) = *sgn*(*w* · Φ(*x*) + *b*)**

QP with Quintic basis functions

We must do $R^2/2$ dot products to get this matrix ready.

In 100-d, each dot product now needs 103 operations instead of 75 million

But there are still worrying things lurking away. What are they?

$$Q_{kl} = y_k y_l(\mathbf{\Phi}(\mathbf{x}_k).\mathbf{\Phi}(\mathbf{x}_l))$$

The use of Maximum Margin magically makes this not a problem

constraints: $\forall k$ $\quad \sum_k \alpha_k y_k = 0$

•The fear of overfitting with this enormous number of terms

•The evaluation phase (doing a set of predictions on a test set) will be very expensive (why?)

Then define:

$$\mathbf{w} = \sum_k \alpha_k y_k \mathbf{\Phi}(\mathbf{x}_k)$$

Because each $\mathbf{w}\cdot\Phi(\mathbf{x})$ (see below) needs 75 million operations. What can be done?

$$\mathbf{w}\cdot\mathbf{\Phi}(\mathbf{x}) = \sum_{k \text{ s.t. } \alpha_k > 0} \alpha_k y_k \mathbf{\Phi}(\mathbf{x}_k)\cdot\mathbf{\Phi}(\mathbf{x})$$
$$= \sum_{k \text{ s.t. } \alpha_k > 0} \alpha_k y_k (\mathbf{x}_k \cdot \mathbf{x} + 1)^5$$

Only *Sm* operations (*S* = # support vectors)

When you see this many callout bubbles on a slide it's time to wrap the author in a blanket, gently take him away and murmur "someone's been at the PowerPoint for too long."

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QP with Quintic basis functions

Maximize $\sum_{k=1}^{R} \alpha_k + \sum_{k=1}^{R} \sum_{l=1}^{R} \alpha_k \alpha_l Q_{kl}$ wh

Andrew's opinion of why SVMs don't overfit as much as you'd think:

No matter what the basis function, there are really only up to R parameters: α_1, α_2 .. α_R, and usually most are set to zero by the Maximum Margin.

Asking for small **w·w** is like "weight decay" in Neural Nets and like Ridge Regression parameters in Linear regression and like the use of Priors in Bayesian Regression---all designed to smooth the function and reduce overfitting.

Subject to these constraints: $0 \le \alpha_k \le C$

Then define:

$$\mathbf{w} = \sum_k \alpha_k y_k \mathbf{\Phi}(\mathbf{x}_k)$$

$$\mathbf{w} \cdot \mathbf{\Phi}(\mathbf{x}) = \sum_{k \text{ s.t. } \alpha_k > 0} \alpha_k y_k \mathbf{\Phi}(\mathbf{x}_k) \cdot \mathbf{\Phi}(\mathbf{x})$$
$$= \sum_{k \text{ s.t. } \alpha_k > 0} \alpha_k y_k (\mathbf{x}_k \cdot \mathbf{x} + 1)^5$$

Only *Sm* operations (*S* = # support vectors)

Then classify with:

f(***x***,***w***,*b*) = *sgn*(***w*** · Φ(***x***) + *b*)

The kernel trick revealed

- A nonlinear SVM is just a straightforward generalization of the approach in which standard dot products $\mathbf{x} \cdot \mathbf{z}$ are replaced by more general kernel functions

$$K(\mathbf{x}, \mathbf{z}) = \mathbf{\Phi}(\mathbf{x}) \cdot \mathbf{\Phi}(\mathbf{z})$$

  representing dot products in a higher-dimensional space.
- The beauty of the "kernel trick" is that everything can be computed in terms of this kernel function *K.* The nonlinear embedding $\mathbf{\Phi}$ itself never has to be computed or represented.
- Nor is the weight vector ***w*** explicitly represented or used in any computations.

The kernel trick revealed (cont.)

- The bias weight *b* is computed as follows, where *i* is any index for which $0 < \alpha_i < C$:

$$\begin{aligned} b &= y_i - \Phi(\mathbf{x}_i) \cdot \mathbf{w} \\ &= y_i - \Phi(\mathbf{x}_i) \cdot \sum_k \alpha_k y_k \Phi(\mathbf{x}_k) \\ &= y_i - \sum_k \alpha_k y_k \Phi(\mathbf{x}_k) \cdot \Phi(\mathbf{x}_i) \\ &= y_i - \sum_k \alpha_k y_k K(\mathbf{x}_k, \mathbf{x}_i) \end{aligned}$$

- In practice, for numerical stability, this computation is done for all such *i* and *b* is then taken to be the average.

SVM Kernel Functions

- *K(**a**,**b**)=(**a** · **b** +1)^d^* is one example of an SVM Kernel Function
- Beyond polynomials there are other very high dimensional basis functions that can be made practical by finding the right Kernel Function
  - Radial-Basis-style Kernel Function:

$$K(\mathbf{a},\mathbf{b}) = \exp\left(-\frac{(\mathbf{a}-\mathbf{b})^2}{2\sigma^2}\right)$$

  - Neural-net-style Kernel Function:

$$K(\mathbf{a},\mathbf{b}) = \tanh(\kappa \mathbf{a}.\mathbf{b} - \delta)$$

σ, κ and δ are magic parameters that must be chosen by a model selection method such as CV or VCSRM*

*see VC-dim lecture

- Choosing kernel function = main design decision

VC-dimension of an SVM

- Very very very loosely speaking there is some theory which under some different assumptions puts an upper bound on the VC dimension as

$$\left\lceil \frac{\text{Diameter}}{\text{Margin}} \right\rceil$$

- where
  - *Diameter* is the diameter of the smallest sphere that can enclose all the high-dimensional term-vectors derived from the training set.
  - *Margin* is the smallest margin we'll let the SVM use
- This can be used in SRM (Structural Risk Minimization) for choosing the polynomial degree, RBF σ, etc.
  - But most people just use Cross-Validation

SVM Performance

- Anecdotally they work very very well indeed.
- Example: They are currently the best-known classifier on a well-studied hand-written-character recognition benchmark
- Another Example: Andrew knows several reliable people doing practical real-world work who claim that SVMs have saved them when their other favorite classifiers did poorly.
- There is a lot of excitement and religious fervor about SVMs as of 2001.

Doing multi-class classification

- SVMs can only handle two-class outputs (i.e. a categorical output variable with arity 2).
- What can be done?
- Answer: with output arity N, learn N SVM's
  - SVM 1 learns "Output==1" vs "Output != 1"
  - SVM 2 learns "Output==2" vs "Output != 2"
  - :
  - SVM N learns "Output==N" vs "Output != N"
- Then to predict the output for a new input, just predict with each SVM and find out which one puts the prediction the furthest into the positive region.

References

- An excellent tutorial on VC-dimension and Support Vector Machines:

C.J.C. Burges. A tutorial on support vector machines for pattern recognition. Data Mining and Knowledge Discovery, 2(2):955-974, 1998. http://citeseer.nj.nec.com/burges98tutorial.html

- The VC/SRM/SVM Bible:

Statistical Learning Theory by Vladimir Vapnik, Wiley-Interscience; 1998

What You Should Know

- Linear SVMs
- The definition of a maximum margin classifier
- What QP can do for you (but not how QP solutions are computed)
- How Maximum Margin can be turned into a QP problem
- How we deal with noisy (non-separable) data
- How we permit non-linear boundaries
- How SVM Kernel functions permit us to pretend we're working with ultra-high-dimensional basis-function terms

