Support Vector Machines

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Cs540 section 2

Announcements

- Projects Due Today
  - I'll put links on course website tomorrow.
  - Check out projects Courses before next week
- Presentations next Week
  - 15 minutes total
    - Leave a few minutes for questions
  - 5 teams each day
  - Presentations In order as they appear on website
  - Email me any slides you want to use (or bring your own laptop)
  - Questions on final may be taken from presentations or project web-sites

Annoucements

- Things left in the course:
  - Presentations next week
  - Evaluate each-others projects (week after presentations)
  - 2 more lectures after presentations
- Reading:
  - Chapter 20 section 6 and 7 on Support Vector Machines

Things You Should Know

- In Depth
  - K-NN, Decision Trees, Perceptron, Neural Network, Ensembles, Naïve Bayes, Bayesian Network, K-Means clustering
  - Induction
  - Inference
  - How they Divide up feature space
  - Important aspects of each model

Things You Should Know

- Overview
  - Inductive Logic Programming
    - FOIL
    - PROGOL
    - GOLEM
  - Support Vector Machines
  - Re-enforcement Learning
    - Q-Learning
- Understand the important points of each model
  - When are they used, how are the models more or less expressive
  - Important terms
  - General Idea of how the algorithm works

What is a Support Vector Machine?

- An optimally defined surface
- Typically nonlinear in the input space
- Linear in a higher dimensional space
- Implicitly defined by a kernel function

Acknowledgments: These slides combine and modify ones provided by Andrew Moore (CMU), Glenn Fung (Wisconsin), and Olvi Mangasarian (Wisconsin), and Chuck Dyer (Wisconsin)

What are Support Vector Machines Used For?

- Classification
- Regression and data-fitting
- Supervised and unsupervised learning

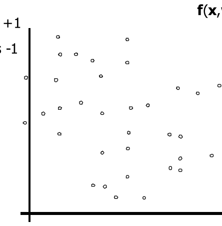
Linear Classifiers

x → f → y

f(**x**,**w**,b) = sign(**w** · **x** + b)

° denotes +1

° denotes -1



How would you classify this data?

Linear Classifiers

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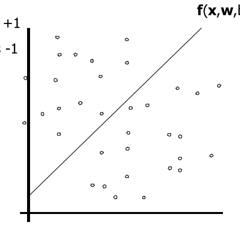

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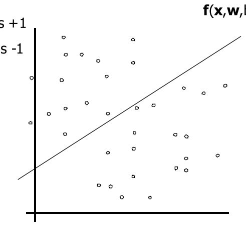

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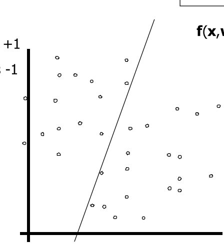

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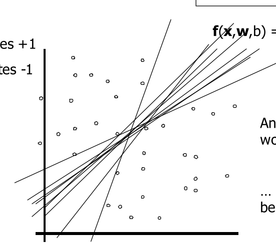
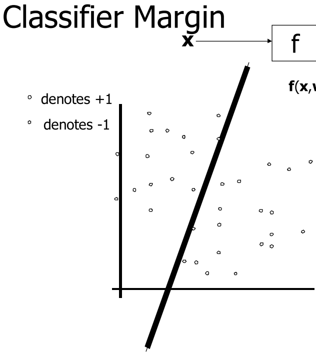


Any of these would be fine ...

... but which is best?

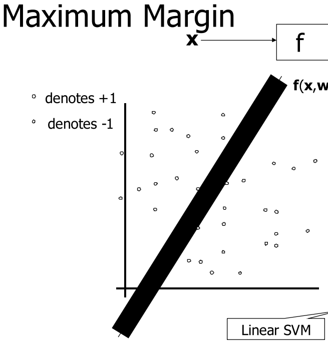
Classifier Margin



f(**x**,**w**,b) = sign(**w** · **x** + b)

Define the margin of a linear classifier as the width that the boundary could be increased by before hitting a data point

Maximum Margin

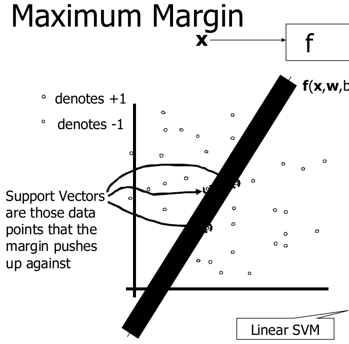


f(**x**,**w**,b) = sign(**w** · **x** + b)

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



f(**x**,**w**,b) = sign(**w** · **x** + b)

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

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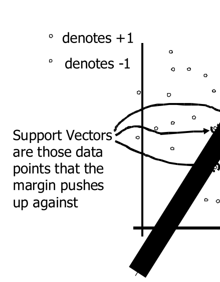
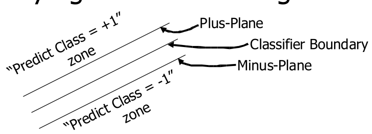
Why Maximum Margin?



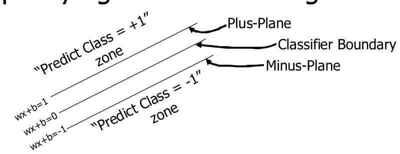
1. Intuitively this feels safest
2. If we've made a small error in the location of the boundary (it's been jolted in its perpendicular direction) this gives us least chance of causing a misclassification
3. Robust to outliers since the model is immune to change/removal of any non-support-vector data points
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 well

Specifying a Line and Margin



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

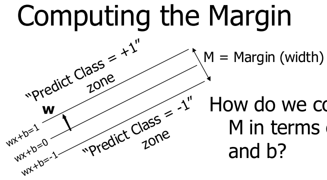
Specifying a Line and Margin



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

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

Computing the Margin

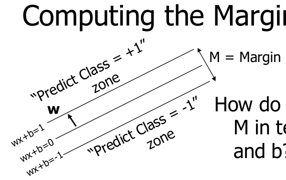


How do we compute M in terms of **w** and b?

- Plus-plane = { **w x** + b = +1 }
- Minus-plane = { **w x** + b = -1 }

Claim: The vector **w** is perpendicular to the Plus-Plane

Computing the Margin



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

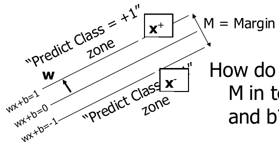
- Plus-plane = { **w x** + b = +1 }
- Minus-plane = { **w x** + b = -1 }

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

Let **u** and **v** be two vectors on the Plus Plane. What is **w** . (**u** – **v**) ?

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

Computing the Margin

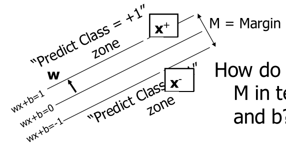


How do we compute M in terms of **w** and b?

- Plus-plane = { **w x** + b = +1 }
- Minus-plane = { **w x** + b = -1 }
- 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

Computing the Margin



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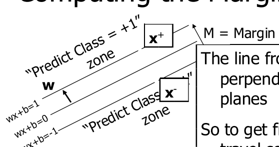
- Claim: $\mathbf{x}^+ = \mathbf{x}^- + \lambda\, \mathbf{w}$ for some value of λ. Why?

Computing the Margin



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

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

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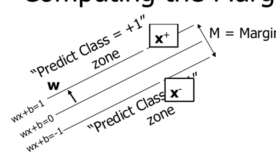
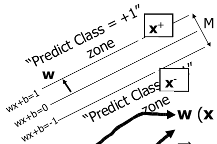


What we know:

- $\mathbf{w}\,\mathbf{x}^+ + b = +1$
- $\mathbf{w}\,\mathbf{x}^- + b = -1$
- $\mathbf{x}^+ = \mathbf{x}^- + \lambda\, \mathbf{w}$
- $|\mathbf{x}^+ - \mathbf{x}^-| = M$

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

Computing the Margin



What we know:

- $\mathbf{w}\,\mathbf{x}^+ + b = +1$
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- $\mathbf{x}^+ = \mathbf{x}^- + \lambda\,\mathbf{w}$
- $|\mathbf{x}^+ - \mathbf{x}^-| = M$

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

$\mathbf{w}\,(\mathbf{x}^- + \lambda\,\mathbf{w}) + b = 1$

$\Rightarrow$

$\mathbf{w}\,\mathbf{x}^- + b + \lambda\,\mathbf{w}\mathbf{w} = 1$

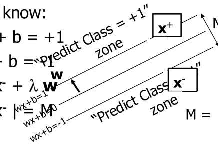
$\Rightarrow$

$-1 + \lambda\,\mathbf{w}\mathbf{w} = 1$

$\Rightarrow$

$$\lambda = \frac{2}{\mathbf{w}.\mathbf{w}}$$

Computing the Margin



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-

$$\lambda = \frac{2}{\mathbf{w}.\mathbf{w}}$$

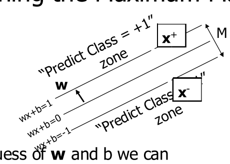
$M = |\mathbf{x}^+ - \mathbf{x}^-| = |\lambda\,\mathbf{w}| =$

$$= \lambda\,|\mathbf{w}| = \lambda\sqrt{\mathbf{w}.\mathbf{w}}$$

$$= \frac{2\sqrt{\mathbf{w}.\mathbf{w}}}{\mathbf{w}.\mathbf{w}} = \frac{2}{\sqrt{\mathbf{w}.\mathbf{w}}}$$

$$= \frac{2}{\|w\|}$$

Learning the Maximum Margin Classifier



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

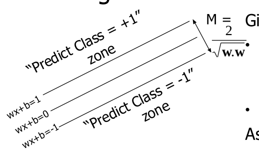
- Compute whether all data points in the correct half-planes
- Compute the width of the margin

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 data points. How?

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

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

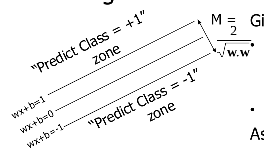
Assume R datapoints, each ($\mathbf{x}_k$, y_k) where y_k = +/- 1

What should our quadratic optimization criterion be?

How many constraints will we have?

What should they be?

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 data points, each ($\mathbf{x}_k$, y_k) where y_k = +/- 1

What should our quadratic optimization criterion be?

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

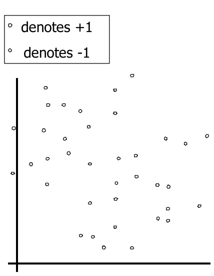
How many constraints will we have? R

What should they be?

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

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

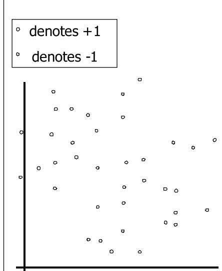
Uh-oh!



This is going to be a problem!

What should we do?

Uh-oh!



This is going to be a problem!

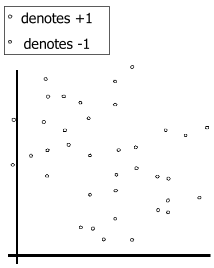
What should we do?

Idea 1:

Find minimum $||\mathbf{w}||^2$, while minimizing number of training set errors

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

Uh-oh!



This is going to be a problem!

What should we do?

Idea 1.1:

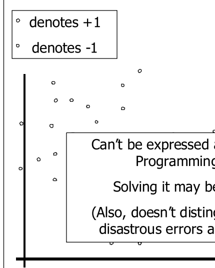
Minimize

$||\mathbf{w}||^2 + C$ (#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

$||\mathbf{w}||^2 + C$ (#train errors)

Tradeoff parameter

Can't be expressed as a Quadratic Programming problem.

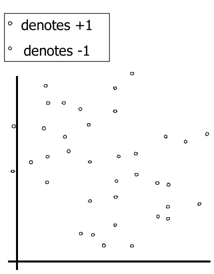
Solving it may be too slow.

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

There's a serio… us reject thi… you guess wh…

So… any other ideas?

Uh-oh!



This is going to be a problem!

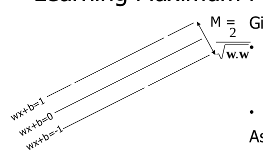
What should we do?

Idea 2.0:

Minimize

$||\mathbf{w}||^2 + C$ (distance of error points to their correct place)

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

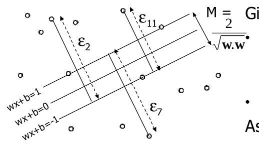
Assume R datapoints, each ($\mathbf{x}_k$, y_k) where y_k = +/- 1

What should our quadratic optimization criterion be?

How many constraints will we have?

What should they be?

Learning Maximum Margin with Noise



$M = \frac{2}{\sqrt{\mathbf{w}.\mathbf{w}}}$

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

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

Assume R datapoints, each ($\mathbf{x}_k$, y_k) where y_k = +/- 1

What should our quadratic optimization criterion be?

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

How many constraints will we have? R

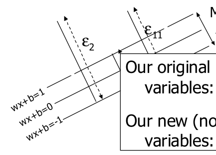
What should they be?

w . $\mathbf{x}_k$ + b >= 1-ε_k if y_k = 1

w . $\mathbf{x}_k$ + b <= -1+ε_k if y_k = -1

Learning Maximum Margi… …oise

m = # input dimensions



$M = \frac{2}{\sqrt{\mathbf{w}.\mathbf{w}}}$

Given gu… …we can

- Compute sum of distances

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

Our new (noisy data) QP has m+1+R variables: w_1, w_2, … w_m, b, ε_k , ε_1 ,… ε_R

R= # records

What should our quadratic optimization criterion be?

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

How many constraints will we have? R

What should they be?

w . $\mathbf{x}_k$ + b >= 1-ε_k if y_k = 1

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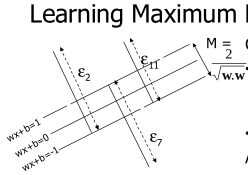
Learning Maximum Margin with Noise



$M = \frac{2}{\sqrt{\mathbf{w}.\mathbf{w}}}$

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

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

Assume R datapoints, each ($\mathbf{x}_k$,y_k) where y_k = +/- 1

What should our quadratic optimization criterion be?

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

How many constraints will we have? R

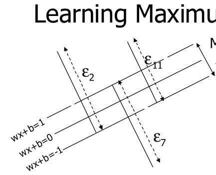
What should they be?

w . $\mathbf{x}_k$ + b >= 1-ε_k if y_k = 1

w . $\mathbf{x}_k$ + b <= -1+ε_k if y_k = -1

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

Learning Maximum Margin with Noise



$M = \frac{2}{\sqrt{\mathbf{w}.\mathbf{w}}}$

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

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

Assume R datapoints, each ($\mathbf{x}_k$,y_k) where y_k = +/- 1

What should our quadratic optimization criterion be?

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

How many constraints will we have? 2R

What should they be?

w . $\mathbf{x}_k$ + b >= 1-ε_k if y_k = 1

w . $\mathbf{x}_k$ + b <= -1+ε_k if y_k = -1

ε_k >= 0 for all k

An Equivalent QP

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

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:

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

$$b = y_K (1 - \varepsilon_K) - \mathbf{x}_K . \mathbf{w}_K$$

$$\text{where } K = \arg\max_k \alpha_k$$

Then classify with:

f(**x**,**w**,b) = sign(**w. 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 $Q_{kl} = y_k y_l (\mathbf{x}_k . \mathbf{x}_l)$

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

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

Then define:

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

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

$$b = y_K (1 - \varepsilon_K) - \mathbf{x}_K . \mathbf{w}_K$$

$$\text{where } K = \arg\max_k \alpha_k$$

Then classify with:

f(**x**,**w**,b) = sign(**w. x** - b)

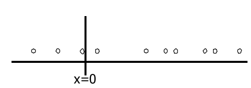
An Equivalent QP

Why did I tell you about this equivalent QP?

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

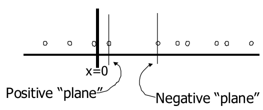
Suppose we're in 1 Dimension

What would SVMs do with this data?



Suppose we're in 1 Dimension

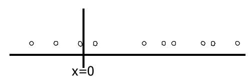
Not a big surprise



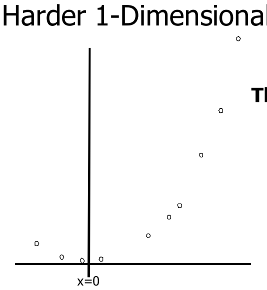
Harder 1-Dimensional Dataset

That's wiped the smirk off SVM's face

What can be done about this?



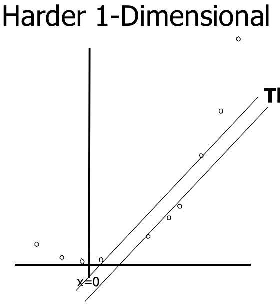
Harder 1-Dimensional Dataset



The Kernel Trick: Preprocess the data, mapping **x** into higher dimensional space **F**(**x**)

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

Harder 1-Dimensional Dataset

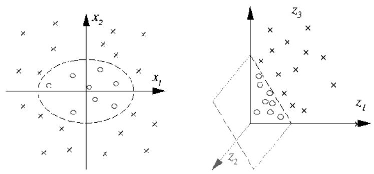


The Kernel Trick: Preprocess the data, mapping **x** into higher dimensional space **F**(**x**)

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

Example: All Degree 2 Monomials

$$\Phi : \mathbb{R}^2 \to \mathbb{R}^3$$
$$(x_1, x_2) \mapsto (z_1, z_2, z_3) := (x_1^2, \sqrt{2}x_1x_2, x_2^2)$$



B. Schölkopf, NIPS, 3 December 2001

- Project examples into some higher dimensional space where the data is linearly separable, defined by $\mathbf{z} = \mathbf{F}(\mathbf{x})$
- Training depends only on dot products of the form $\mathbf{F}(\mathbf{x}_i) \cdot \mathbf{F}(\mathbf{x}_j)$
- Example:

$$F(x) = (x_1^2, \sqrt{2}x_1x_2, x_2^2)$$

$$\mathbf{K}(\mathbf{x}_i, \mathbf{x}_j) = \mathbf{F}(\mathbf{x}_i) \cdot \mathbf{F}(\mathbf{x}_j) = (\mathbf{x}_i \cdot \mathbf{x}_j)^2$$

Common SVM Basis Functions

$\mathbf{z}_k$ = (polynomial terms of $\mathbf{x}_k$ of degree 1 to q)

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

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

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

SVM Kernel Functions

- $K(\mathbf{a},\mathbf{b})=(\mathbf{a} \,.\, \mathbf{b} + 1)^d$ is an 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

The Federalist Papers

- Written in 1787-1788 by Alexander Hamilton, John Jay, and James Madison to persuade the citizens of New York to ratify the constitution
- Papers consisted of short essays, 900 to 3500 words in length
- Authorship of 12 of those papers have been in dispute (Madison or Hamilton); these papers are referred to as the disputed Federalist papers

Description of the Data

- For every paper:
  - Machine readable text was created using a scanner
  - Computed relative frequencies of 70 words that Mosteller-Wallace identified as good candidates for author-attribution studies
  - Each document is represented as a vector containing the 70 real numbers corresponding to the 70 word frequencies
- The dataset consists of 118 papers:
  - 50 Madison papers
  - 56 Hamilton papers
  - 12 disputed papers

Function Words Based on Relative Frequencies

1	*a*	15	*do*	29	*is*	43	*or*	57	*this*
2	*all*	16	*down*	30	*it*	44	*our*	58	*to*
3	*also*	17	*even*	31	*its*	45	*shall*	59	*up*
4	*an*	18	*every*	32	*may*	46	*should*	60	*upon*
5	*and*	19	*for*	33	*more*	47	*so*	61	*was*
6	*any*	20	*from*	34	*must*	48	*some*	62	*were*
7	*are*	21	*had*	35	*my*	49	*such*	63	*what*
8	*as*	22	*has*	36	*no*	50	*than*	64	*when*
9	*at*	23	*have*	37	*not*	51	*that*	65	*which*
10	*be*	24	*her*	38	*now*	52	*the*	66	*who*
11	*been*	25	*his*	39	*of*	53	*their*	67	*will*
12	*but*	26	*if*	40	*on*	54	*then*	68	*with*
13	*by*	27	*in*	41	*one*	55	*there*	69	*would*
14	*can*	28	*into*	42	*only*	56	*things*	70	*your*

SLA Feature Selection for Classifying the Disputed Federalist Papers

- Apply the SVM Successive Linearization Algorithm for feature selection to:
  - Train on the 106 Federalist papers with known authors
  - Find a classification hyperplane that uses as few words as possible
- Use the hyperplane to classify the 12 disputed papers

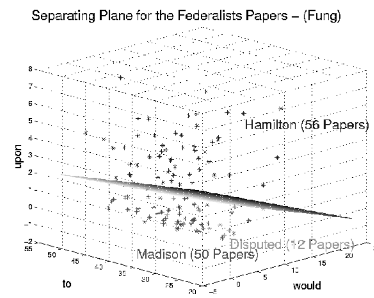
Hyperplane Classifier Using 3 Words

- A hyperplane depending on three words was found:

$$0.537to + 24.663upon + 2.953would = 66.616$$

- All disputed papers ended up on the Madison side of the plane

Results: 3D Plot of Hyperplane



Multi-Class Classification

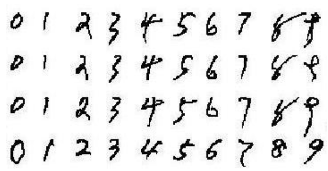
- SVMs can only handle two-class outputs
- What can be done?
- Answer: for N-class problems, learn N SVM's:
  - SVM 1 learns "Output=1" vs "Output ≠ 1"
  - SVM 2 learns "Output=2" vs "Output ≠ 2"
  - :
  - SVM N learns "Output=N" vs "Output ≠ N"
- To predict the output for a new input, just predict with each SVM and find out which one puts the prediction the furthest into the positive region

Summary

- Learning linear functions
  - Pick separating plane that maximizes margin
  - Separating plane defined in terms of support vectors only
- Learning non-linear functions
  - Project examples into higher dimensional space
  - Use kernel functions for efficiency
- Generally avoids over-fitting problem
- Global optimization method; no local optima
- Can be expensive to apply, especially for multi-class problems

Case Study

- Handwritten digits important domain
  - Automated sorting of mail (zip code recognition)
- NIST dataset of handwritten digits
  - 60,000 labeled digits, 20x20=400 pixels in 8-bit greyscale values



Case Study -- Models

- 3 Nearest Neighbor
- ANN with 300 hidden units
- ANN specially crafted for the domain (LeNet)
  - Lots of work went into crafting this
- LeNet with Ensembles (Boosted LeNet)
- SVM (almost no effort in creating the model)
- Virtual SVM (specially crafted for the domain)
- Shape Matching instead of standard distance in 3NN
- Human (somewhere in the range of 0.2% error rate and 2.5% error rate)

Case Study Results

	3 NN	300 Hidden	LeNet	Boosted LeNet	SVM	Virtual SVM	Shape Match
Error Rate	2.4%	1.6%	0.9%	0.7%	1.1%	0.56%	0.63%
Runtime (ms/digit)	1000	10	30	50	2000	200	
Memory (MB)	12	.49	.012	.21	11		
Training time (days)	0	7	14	30	10		
% rejected to reach 0.5% accuracy	8.1%	3.2%	1.8%	0.5%	1.8%		