Supervised Learning Methods

- k-nearest-neighbors
- Decision trees
- Neural networks
- Naïve Bayes
- **Support vector machines (SVM)**

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Support Vector Machines

Chapter 18.9 and the optional paper "Support vector machines" by M. Hearst, ed., 1998

Acknowledgments: These slides combine and modify ones provided by Andrew Moore (CMU), Carla Gomes (Cornell), Mingyue Tan (UBC), Jerry Zhu (Wisconsin), Glenn Fung (Wisconsin), and Olvi Mangasarian (Wisconsin)

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What are Support Vector Machines (SVMs) Used For?

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

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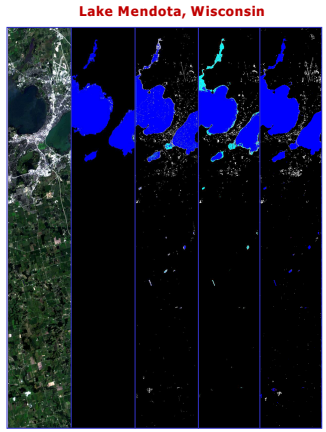
Lake Mendota, Madison, WI

- Identify areas of land cover (land, ice, water, snow) in a scene
- Two methods:
  - Scientist manually-derived
  - Support Vector Machine (SVM)

Classifier	Expert Derived	SVM
cloud	45.7%	58.5%
ice	60.1%	80.4%
land	93.6%	94.0%
snow	63.5%	71.6%
water	84.2%	89.1%
unclassified	45.7%	

Courtesy of Steve Chien of NASA/JPL



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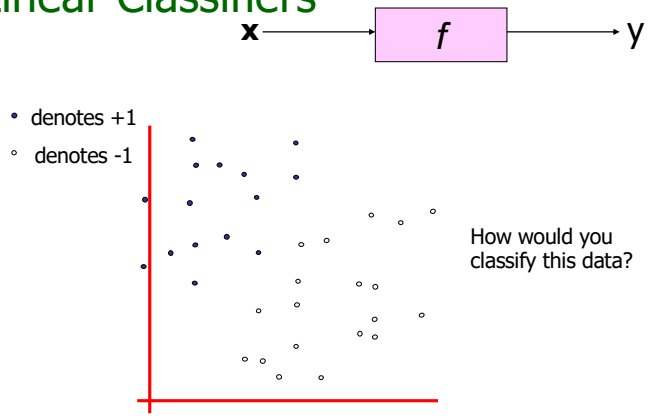
Linear Classifiers



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Linear Classifiers (aka Linear Discriminant Functions)

- Definition:

  A function that is a linear combination of the components of the input (column vector) **x**:

$$f(\mathbf{x}) = \sum_{j=1}^{d} w_j x_j + b = \mathbf{w}^{\mathrm{T}}\mathbf{x} + b$$

  where **w** is the weight (column vector) and *b* is the bias

- A **2-class classifier** then uses the rule:

  Decide class c_1 if $f(\mathbf{x}) \geq 0$ and class c_2 if $f(\mathbf{x}) < 0$

  or, equivalently, decide c_1 if $\mathbf{w}^{\mathrm{T}}\mathbf{x} \geq -b$ and c_2 otherwise

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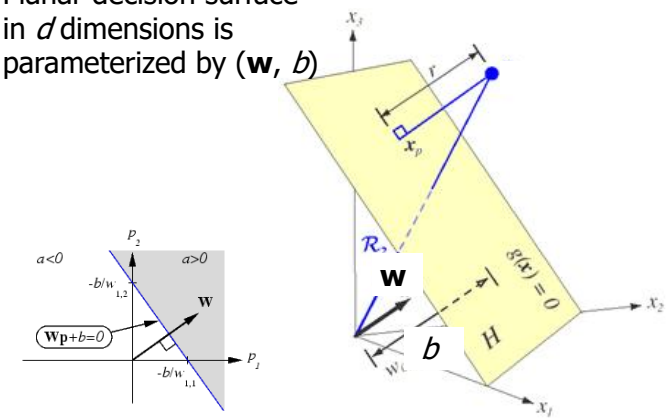
Planar decision surface in *d* dimensions is parameterized by (**w**, *b*)

w is the plane's normal vector

b is the distance from the origin



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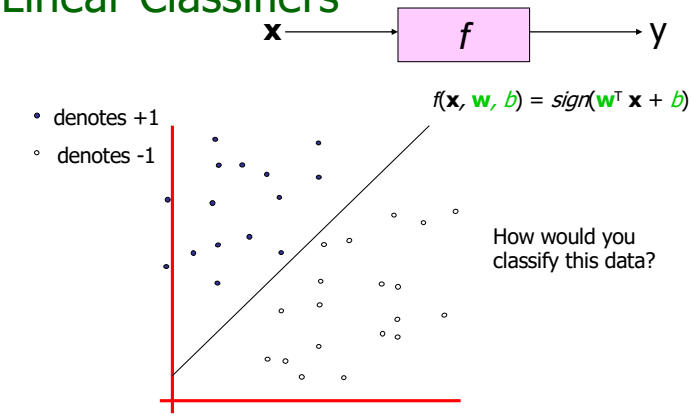
Linear Classifiers



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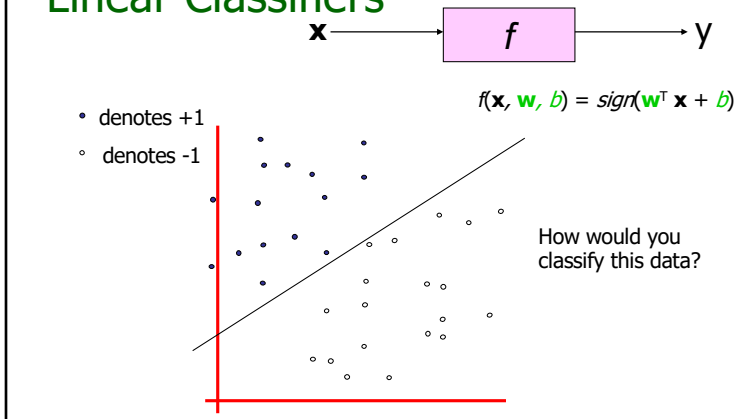
Linear Classifiers



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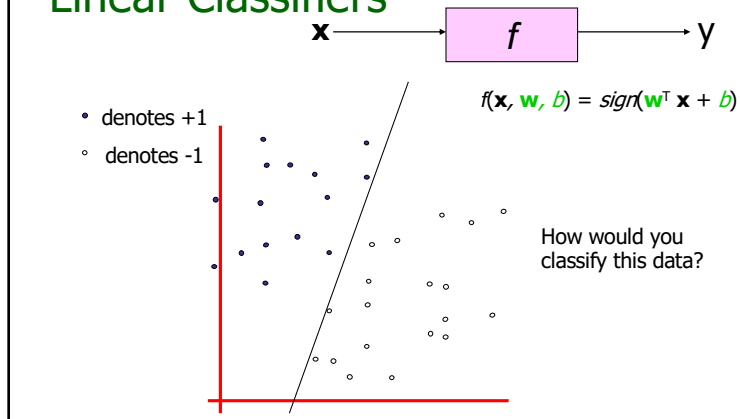
Linear Classifiers



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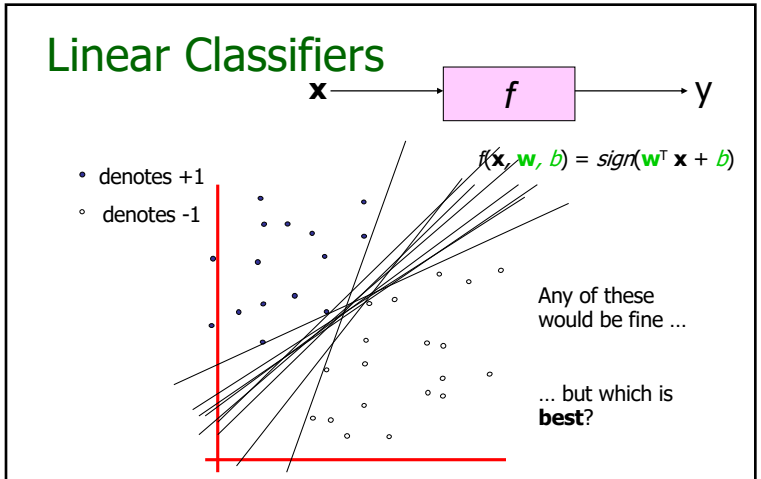
Linear Classifiers



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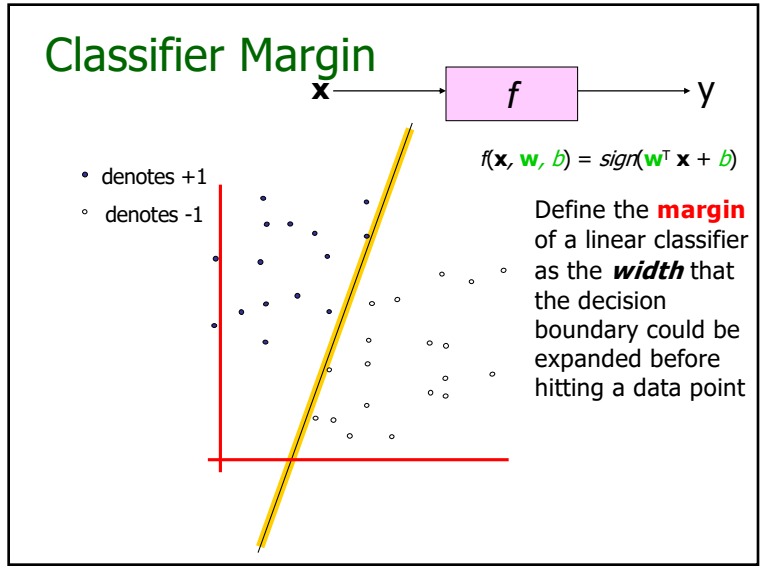
Classifier Margin



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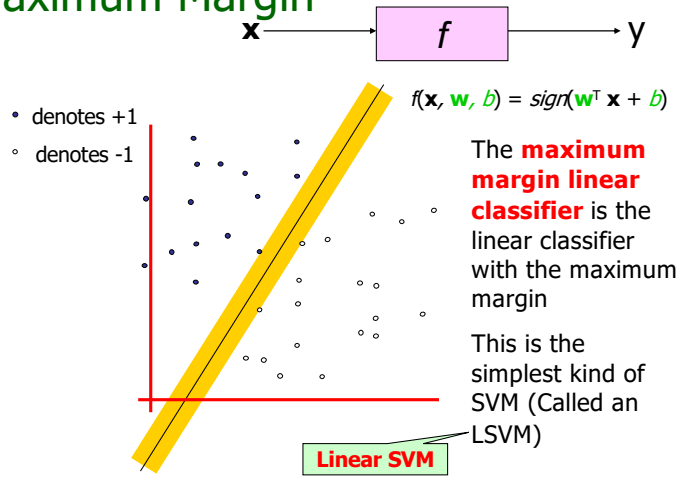
Maximum Margin



The **maximum margin linear classifier** is the linear classifier with the maximum margin

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

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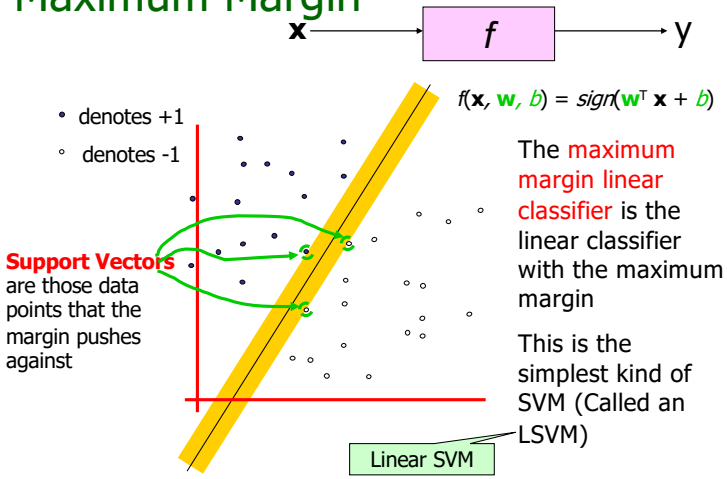
Maximum Margin



The maximum margin linear classifier is the linear classifier with the maximum margin

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

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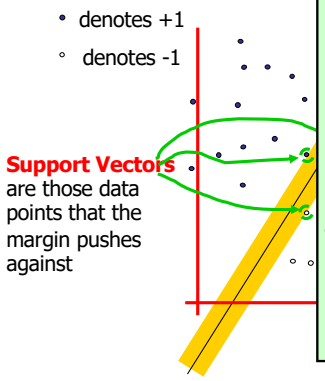
Why the Maximum Margin?



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*

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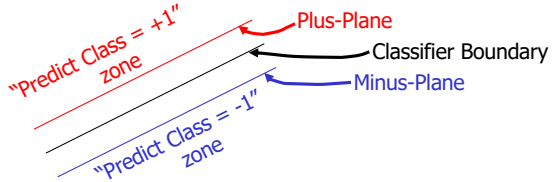
Specifying a Line and Margin



- How do we represent this mathematically?
- … in *d* input dimensions?
- An example $\mathbf{x} = (x_1, \ldots, x_d)^T$

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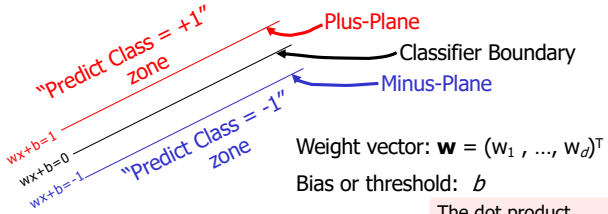
Specifying a Line and Margin



Weight vector: $\mathbf{w} = (w_1, \ldots, w_d)^T$

Bias or threshold: b

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

The dot product $\mathbf{w}^T \cdot \mathbf{x} = \sum_{j=1}^{d} w_j x_j$ is a scalar: $\mathbf{x}$'s projection onto $\mathbf{w}$

Classify as +1 if $\mathbf{w}^T \mathbf{x} + b \geq 1$

-1 if $\mathbf{w}^T \mathbf{x} + b \leq -1$

? if $-1 < \mathbf{w}^T \mathbf{x} + b < 1$

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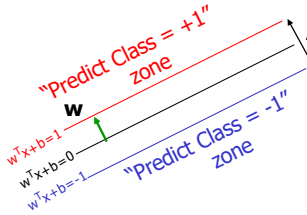
Computing the Margin



How do we compute M in terms of $\mathbf{w}$ and b?

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

Claim: The vector $\mathbf{w}$ is perpendicular to the Plus-Plane and the Minus-Plane

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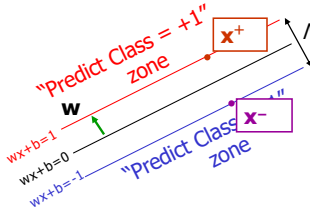
Computing the Margin



How do we compute M in terms of $\mathbf{w}$ and b?

- Plus-plane = $\mathbf{w}^T \mathbf{x} + b = +1$
- Minus-plane = $\mathbf{w}^T \mathbf{x} + b = -1$
- The vector $\mathbf{w}$ 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 $\mathbb{R}^d$; not necessarily a data point

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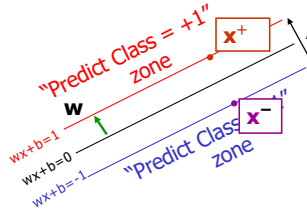
Computing the Margin



How do we compute M in terms of $\mathbf{w}$ and b?

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- Let $\mathbf{x}^+$ be the closest Plus-Plane-point to $\mathbf{x}^-$
- Claim: $\mathbf{x}^+ = \mathbf{x}^- + \lambda \mathbf{w}$ for some value of λ

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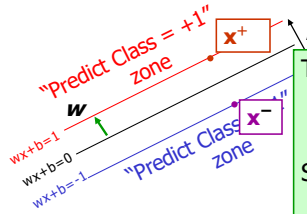
Computing the Margin



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 $\mathbf{w}$

- Plus-plane = $\mathbf{w}^T \mathbf{x} + b = +1$
- Minus-plane = $\mathbf{w}^T \mathbf{x} + b = -1$
- The vector $\mathbf{w}$ 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 $\mathbf{x}^-$
- Claim: $\mathbf{x}^+ = \mathbf{x}^- + \lambda \mathbf{w}$ for some value of λ Why?

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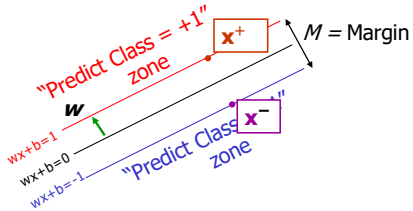
Computing the Margin



What we know:

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

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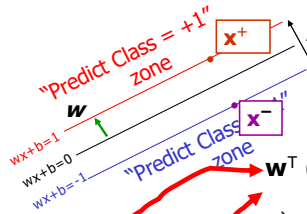
Computing the Margin



What we know:

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

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

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

$\Rightarrow$

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

$\Rightarrow$

$-1 + \lambda \mathbf{w}^T \mathbf{w} = 1$

$\Rightarrow \quad \lambda = \dfrac{2}{\mathbf{w}^T \mathbf{w}}$

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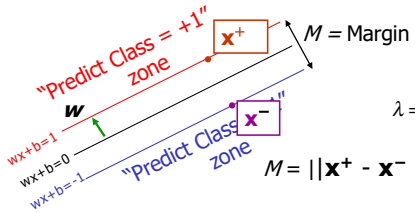
Computing the Margin



What we know:

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

$M = \text{Margin} = \dfrac{2}{\sqrt{\mathbf{w}^T \mathbf{w}}}$

$\lambda = \dfrac{2}{\mathbf{w}^T \mathbf{w}}$

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

$= \lambda \|\mathbf{w}\| = \lambda \sqrt{\mathbf{w}^T \mathbf{w}}$

$= \dfrac{2\sqrt{\mathbf{w}^T \mathbf{w}}}{\mathbf{w}^T \mathbf{w}} = \dfrac{2}{\sqrt{\mathbf{w}^T \mathbf{w}}}$

$= \dfrac{2}{\|\mathbf{w}\|}$ = M, margin size

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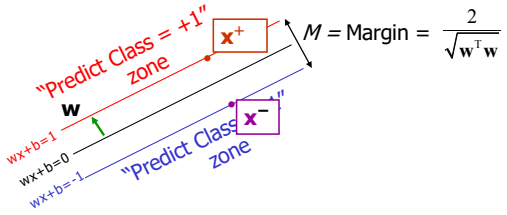
Learning the Maximum Margin Classifier



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

1. Compute whether all data points in the correct half-planes
2. Compute 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 correctly classifies all the data points *How?*

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SVM as Constrained Optimization

- Unknowns: **w**, *b*
- Objective function: maximize the margin:
  $M = 2 / ||\mathbf{w}||$
- Equivalent to **minimizing** $||\mathbf{w}||$ or $||\mathbf{w}||^2 = \mathbf{w}^T\mathbf{w}$

- *N* training points: $(\mathbf{x}_k, y_k)$, $y_k = +1$ or -1
- Subject to each training point correctly classified, i.e.,

  subject to $y_k(\mathbf{w}^T\mathbf{x}_k + b) \geq 1$ for all k — *N* constraints

This is a **quadratic optimization problem (QP)**, which can be solved efficiently

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Classification with SVMs

Given a new point **x**, we can classify it by

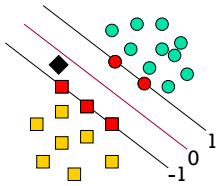
- Computing score: $\mathbf{w}^T\mathbf{x} + b$
- Deciding class based on whether < 0 or > 0

- If desired, can set confidence threshold *t*

Score > *t*: yes

Score < -*t*: no

Else: don't know



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SVMs: More than Two Classes

- **SVMs can only handle two-class problems**
- *k*-class problem: Split the task into *k* **binary** tasks and learn *k* SVMs:
  - Class 1 vs. the rest (classes 2 — *k*)
  - Class 2 vs. the rest (classes 1, 3 — *k*)
  - …
  - Class *k* vs. the rest
- Pick the class that puts the point *farthest into its positive region*

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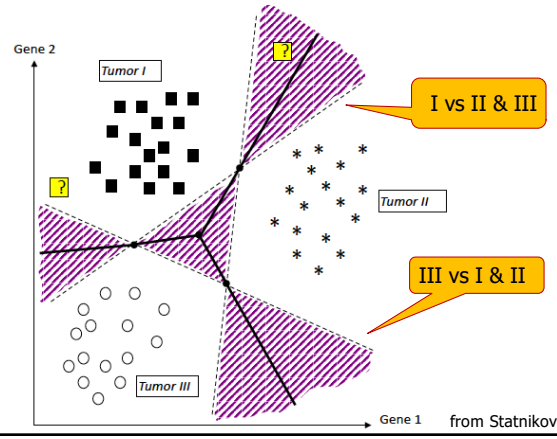
One-versus-rest multicategory SVM method



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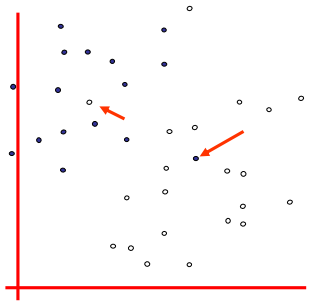
SVMs: Non Linearly-Separable Data

What if the data are ***not*** linearly separable?



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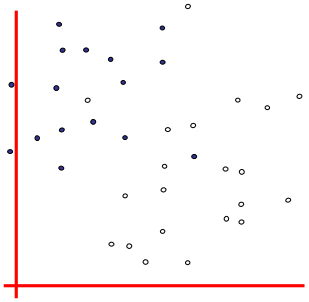
SVMs: Non Linearly-Separable Data

Two approaches:

- Allow a few points on the wrong side (**slack variables**)
- Map data to a higher dimensional space, and do linear classification there (**kernel trick**)



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Non Linearly-Separable Data

Approach 1: Allow a few points on the wrong side (**slack variables**)

"Soft Margin Classification"

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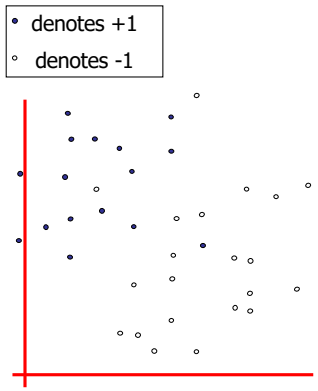
What Should We Do?



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What Should We Do?

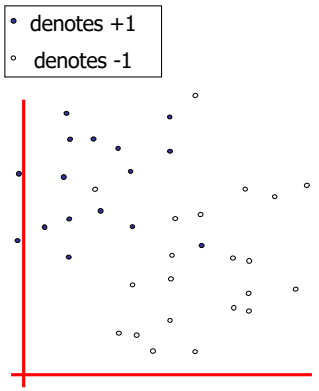
Idea:

Minimize

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

Tradeoff "penalty" parameter

There's a serious practical problem with this approach



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What Should We Do?

Idea:

Minimize

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

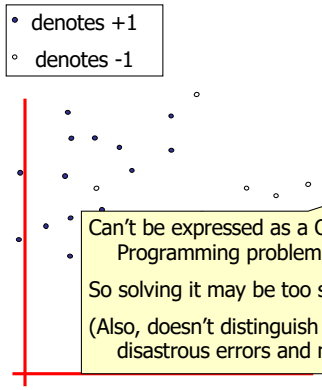
Tradeoff "penalty" parameter

erious practical
th this approach

Can't be expressed as a Quadratic Programming problem.

So solving it may be too slow.

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



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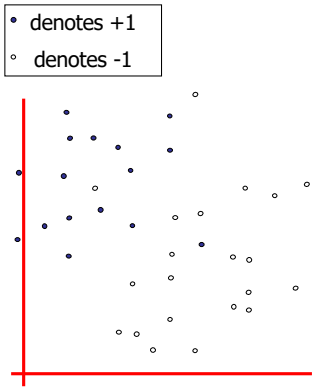
What Should We Do?

Minimize

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



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Choosing *C*, the Penalty Factor

Critical to choose a good value for the constant penalty parameter, *C*, because

- *C* too big means very similar to LSVM because we have a high penalty for non-separable points, and we may use many support vectors and ***overfit***
- *C* too small means we allow many misclassifications in the training data and we may ***underfit***

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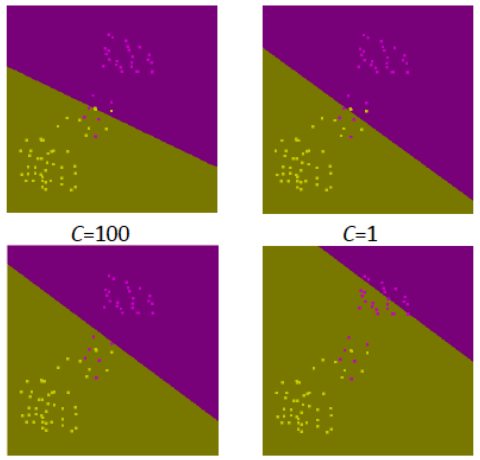
Choosing *C*



from Statnikov et al.

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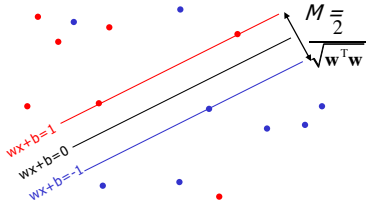
Learning Maximum Margin with Noise



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

1. Compute sum of distances of points to their correct zones
2. Compute the margin width

Assume *N* examples, each ($\mathbf{x}_k$, y_k) where y_k = +1 / -1

What should our optimization criterion be?

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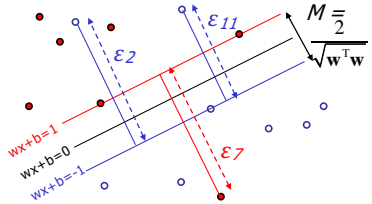
Learning Maximum Margin with Noise



"slack variables"

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

1. Compute sum of distances of points to their correct zones
2. Compute the margin width

Assume *N* examples, each ($\mathbf{x}_k$, y_k) where y_k = +1 / -1

What should our optimization criterion be?

Minimize $\frac{1}{2}\mathbf{w}^{\mathrm{T}}\mathbf{w} + C\sum_{k=1}^{N}\varepsilon_k$

How many constraints will we have? ***N***

What should they be?

$y_k(\mathbf{w}^{\mathrm{T}}x_k + b) \geq 1-\varepsilon_k$ for all k

Note: ε_k = 0 for points in correct zone

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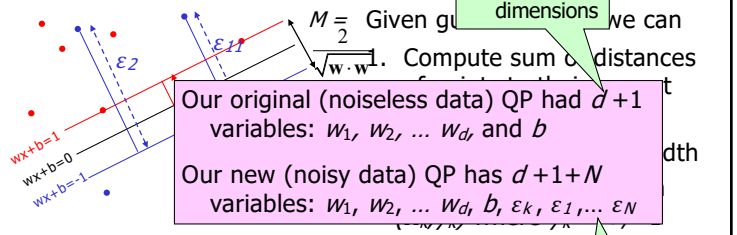
Learning Maximum Margi…ise



$M = \frac{2}{\sqrt{\mathbf{w}\cdot\mathbf{w}}}$ Given gu…we can

1. Compute sum o…distances …t …dth …

d = # input dimensions

Our original (noiseless data) QP had *d* +1 variables: $w_1, w_2, \ldots w_d$ and *b*

Our new (noisy data) QP has *d* +1+*N* variables: $w_1, w_2, \ldots w_d, b, \varepsilon_k, \varepsilon_1, \ldots \varepsilon_N$

N = # examples

What should our optimization criterion be?

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

How many constrai…ll we have? ***N***

What should they be?

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

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

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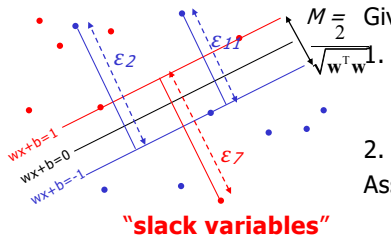
Learning Maximum Margin with Noise



"slack variables"

$M = \frac{2}{\sqrt{\mathbf{w}^T\mathbf{w}}}$ Given guess of **w** , *b* we can

1. Compute sum of distances of points to their correct zones
2. Compute the margin width

Assume *N* examples, each $(\mathbf{x}_k, y_k)$ where y_k = +1 / -1

What should our optimization criterion be?

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

How many constraints will we have? ***2N***

What should they be?

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

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

$\varepsilon_k \geq 0$ for all *k*

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Non Linearly-Separable Data

Approach 2: Map data to a higher dimensional space, and then do linear classification there (called the **kernel trick**)

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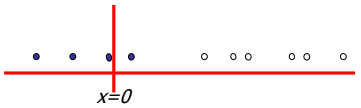
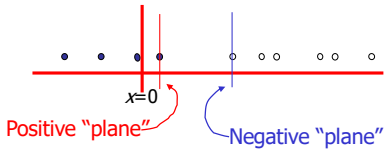
Suppose we're in 1 Dimension

What would SVMs do with this data?



65

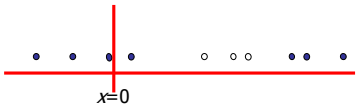
Suppose we're in 1 Dimension



66

Harder 1D Dataset: *Not* Linearly-Separable

What can be done about this?



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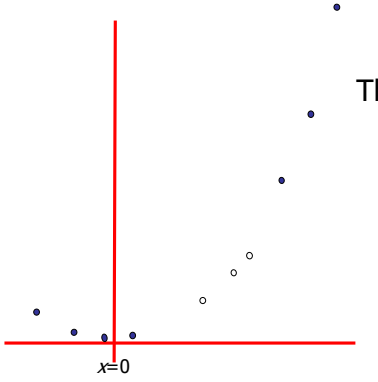
Harder 1D Dataset



The **Kernel Trick**: Preprocess the data, mapping **x** into a higher dimensional space, **z** = Φ(**x**)

For example:

$$\Phi(x) = (x\ , x^2)$$

Here, Φ maps data from 1D to 2D

In general, map from *d*-dimensional input space to *k*-dimensional **z** space

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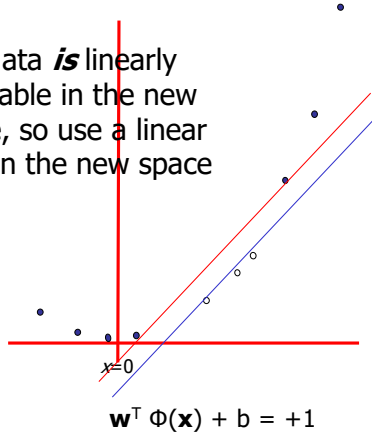
Harder 1D Dataset

The data ***is*** linearly separable in the new space, so use a linear SVM in the new space



The **Kernel Trick**: Preprocess the data, mapping **x** into a higher dimensional space, **z** = Φ(**x**)

$$\Phi(x) = (x\ , x^2)$$

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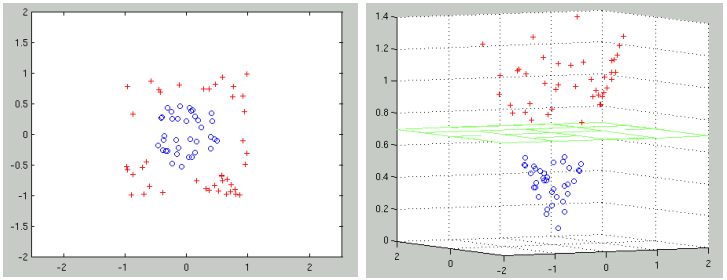
Another Example

$$\Phi(x_1, x_2) = (x_1, x_2, \sqrt{x_1^2 + x_2^2})$$



Project examples into some higher dimensional space where the data ***is*** linearly separable, defined by **z** = Φ(**x**)

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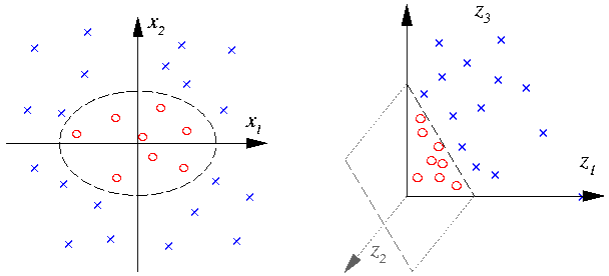
Another Example

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



Project examples into some higher dimensional space where the data ***is*** linearly separable, defined by **z** = Φ(**x**)

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Algorithm

1. Pick a Φ function
2. Map each training example, **x**, into the new higher-dimensional space using **z** = Φ(**x**)
3. Solve the optimization problem using the nonlinearly transformed training examples, **z**, to obtain a Linear SVM (with or without using the slack variable formulation) defined by **w** and *b*
4. Classify a test example, **e**, by computing: *sign*(**w**^{T} · Φ(**e**) + *b*)

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Improving Efficiency

- Time complexity of the original optimization formulation depends on the dimensionality, *k*, of **z** (*k* >> *d*)
- We can convert the optimization problem into an equivalent form, called the *Dual Form*, with time complexity $O(N^3)$ that depends on *N*, the number of training examples, *not k*
- Dual Form will also allow us to rewrite the mapping functions in Φ in terms of "kernel functions" instead

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Dual Optimization Problem

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

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

Then define:

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

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

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

Then classify with:

f(**x**,**w**,*b*) = *sign*(**w**$^{\mathrm{T}}$**x** - *b*)

N examples: ($\mathbf{x}_k$, y_k)
where y_k = +1 / -1

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Dual Optimizatio

Dot product of two examples

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

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

New variables; Examples with $\alpha_k > 0$ will be the support vectors

Then define:

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

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

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

Then classify with:

f(**x**,**w**,*b*) = *sign*(**w**$^{\mathrm{T}}$**x** - *b*)

N examples: ($\mathbf{x}_k$, y_k)
where y_k = +1 / -1

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Algorithm

- Compute *N* x *N* matrix *Q* by computing $y_i y_j (\mathbf{x}_i^{\mathrm{T}} \mathbf{x}_j)$ between *all* pairs of training examples
- Solve the optimization problem to compute α_i
  for *i* = 1, …, N
  - Each non-zero α_i indicates that example $\mathbf{x}_i$ is a support vector
- Compute **w** and b
- Then classify test example **x** with:

  f(**x**) = *sign*(**w**$^{\mathrm{T}}$ **x** – *b*)

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Dual Optimization Problem (After Mapping)

Maximize $\sum_{k=1}^{N} \alpha_k - \frac{1}{2}\sum_{k=1}^{N}\sum_{l=1}^{N} \alpha_k \alpha_l Q_{kl}$ where $Q_{kl} = y_k y_l (\Phi(\mathbf{x}_k)^{\mathrm{T}} \Phi(\mathbf{x}_l))$

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

Then define:

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

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

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

Then classify with:

f(**x**,**w**,*b*) = *sign*(**w**$^{\mathrm{T}}$ Φ(***x***) - *b*)

N examples: ($\mathbf{x}_k$, y_k)
where y_k = +1 / -1

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Dual Optimizzation Problem (After Mapping)

Maximize $\sum_{k=1}^{N}\alpha_k - \frac{1}{2}\sum_{k=1}^{N}\sum_{l=1}^{N}\alpha_k\alpha_l Q_{kl}$ where $Q_{kl} = y_k y_l(\Phi(\mathbf{x}_k)^{\mathrm{T}}\Phi(\mathbf{x}_l))$

Subject to these constraints: $0 \le \alpha_k \le$ *N* (N dot products to compute this matrix) $\sum_{k=1}^{N} y_k = 0$

Then define:

$$\mathbf{w} = \sum_{k \text{ s.t. } \alpha_k > 0} \alpha_k y_k \boldsymbol{\Phi}(\mathbf{x}_k)$$

$$b = y_K(1-\varepsilon_K) - \mathbf{x}_K.\mathbf{w}_K \quad \text{where } K = \arg\max_k \alpha_k$$

Then classify with:

f(**x**,**w**,*b*) = *sign*(**w**$^{\mathrm{T}}$ Φ(**x**) - *b*)

N examples: ($\mathbf{x}_k$, y_k)
where y_k = +1 / -1

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- Dual formulation of the optimization problem depends on the input data only in dot products of the form:
  $\Phi(\mathbf{x}_i)^{\mathrm{T}} \cdot \Phi(\mathbf{x}_j)$ where $\mathbf{x}_i$ and $\mathbf{x}_j$ are two examples
- We can compute these dot products efficiently for certain types of Φ's where $K(\mathbf{x}_i, \mathbf{x}_j) = \Phi(\mathbf{x}_i)^{\mathrm{T}} \cdot \Phi(\mathbf{x}_j)$
- Example:

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

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

- Since the data *only* appears as dot products, we do *not* need to map the data to higher dimensional space (using Φ(**x**)) because we can use the kernel function *K* instead

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

$$\begin{aligned}
&\Phi(x_i)^{\mathrm{T}} \cdot \Phi(x_j) \\
&= x_{i_1}^2 x_{j_1}^2 + \sqrt{2}x_{i_1}x_{i_2}\sqrt{2}x_{j_1}x_{j_2} + x_{i_2}^2 x_{j_2}^2 \\
&= x_{i_1}^2 x_{j_1}^2 + 2x_{i_1}x_{i_2}x_{j_1}x_{j_2} + x_{i_2}^2 x_{j_2}^2 \\
&= (x_{i_1}x_{j_1} + x_{i_2}x_{j_2})^2 \\
&= (x_i^{\mathrm{T}} \cdot x_j)^2
\end{aligned}$$

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Kernel Functions

- A kernel, $K(\mathbf{x}_i, \mathbf{x}_j)$, is a dot product in *some* feature space
- A kernel function is a function that can be applied to pairs of input examples to evaluate dot products in some corresponding (possibly infinite dimensional) feature space
- We do *not* need to compute Φ explicitly

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What's Special about a Kernel?

- Say 1 example (in 2D) is: $\mathbf{s} = (s_1, s_2)$
- We decide to use a particular mapping into 6D space:
  $\Phi(\mathbf{s})^T = (s_1^2, s_2^2, \sqrt{2}s_1s_2, s_1, s_2, 1)$
- Let another example be $\mathbf{t} = (t_1, t_2)$
- Then,

$$\Phi(\mathbf{s})^T \cdot \Phi(\mathbf{t}) = s_1^2 t_1^2 + s_2^2 t_2^2 + 2s_1s_2t_1t_2 + s_1t_1 + s_2t_2 + 1$$
$$= (s_1t_1 + s_2t_2 + 1)^2$$
$$= (\mathbf{s}^T\cdot\mathbf{t} + 1)^2$$

- So, define the **kernel** function to be $K(\mathbf{s}, \mathbf{t}) = (\mathbf{s}^T\cdot\mathbf{t} + 1)^2 = \Phi(\mathbf{s})^T \cdot \Phi(\mathbf{t})$
- We save computation by using kernel K

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Some Commonly Used Kernels

- Linear kernel: $K(\mathbf{x}_i, \mathbf{x}_j) = \mathbf{x}_i^T \mathbf{x}_j$
- Quadratic kernel: $K(\mathbf{x}_i, \mathbf{x}_j) = (\mathbf{x}_i^T \mathbf{x}_j + 1)^2$
- Polynomial of degree d kernel: $K(\mathbf{x}_i, \mathbf{x}_j) = (\mathbf{x}_i^T \mathbf{x}_j + 1)^d$
- Radial-Basis Function (Gaussian) kernel:
  $K(\mathbf{x}_i, \mathbf{x}_j) = \exp(-||\mathbf{x}_i - \mathbf{x}_j||^2 / \sigma^2)$

- Many possible kernels; picking a good one is tricky
- Hacking with SVMs: create various kernels, hope their space Φ is meaningful, plug them into SVM, pick one with good classification accuracy
- Kernel usually combined with slack variables because no guarantee of linear separability in new space

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Algorithm

- Compute N x N matrix Q by computing
  $y_i y_j K(\mathbf{x}_i, \mathbf{x}_j)$ between all pairs of training points
- Solve optimization problem to compute α_i
  for $i = 1, \ldots, N$
  - Each non-zero α_i indicates that example $\mathbf{x}_i$ is a support vector
- Compute $\mathbf{w}$ and b
- Classify test example $\mathbf{x}$ using:
  $f(\mathbf{x}) = sign(\mathbf{w}^T \mathbf{x} - b)$

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Applications of SVMs

- Bioinformatics
- Machine Vision
- Text Categorization
- Ranking (e.g., Google searches)
- Handwritten Character Recognition
- Time series analysis

→ Lots of very successful applications!

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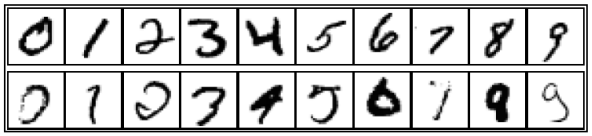
Handwritten Digit Recognition



3-nearest-neighbor = 2.4% error
400–300–10 unit MLP = 1.6% error
LeNet: 768–192–30–10 unit MLP = 0.9% error

Current best (kernel machines, vision algorithms) ≈ 0.6% error

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Example Application: The Federalist Papers Dispute

- Written in 1787-1788 by Alexander Hamilton, John Jay, and James Madison to persuade the citizens of New York to ratify the U.S. 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

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Description of the Data

- For every paper:
  - 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

"Bag of words"

- The dataset consists of 118 papers:
  - 50 Madison papers
  - 56 Hamilton papers
  - 12 disputed papers

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70-Word Dictionary

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*

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Feature Selection for Classifying the Disputed Federalist Papers

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

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Hyperplane Classifier Using 3 Words

- A hyperplane depending on three words was found:

$$0.537\textit{to} + 24.663\textit{upon} + 2.953\textit{would} = 66.616$$

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

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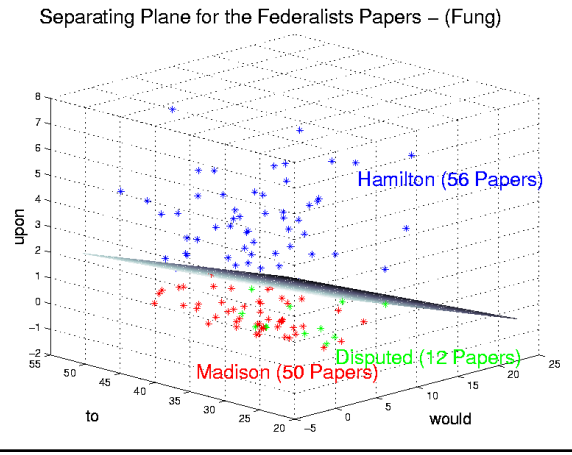
Results: 3D Plot of Hyperplane



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Summary

- Learning linear functions
  - Pick ***separating hyperplane*** that maximizes margin
  - Separating plane defined in terms of support vectors (small number of training examples) *only*
- Learning non-linear functions
  - Project examples into a higher dimensional space
  - Use kernel functions for efficiency
- Generally avoids overfitting problem
- Global optimization method; no local optima
- Can be expensive to apply, especially for multi-class problems
- Biggest Drawback: The choice of kernel function
  - There is no "set-in-stone" theory for choosing a kernel function for any given problem
  - Once a kernel function is chosen, there is only ONE modifiable parameter, the error penalty *C*

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Software

- A list of SVM implementations can be found at `http://www.kernel-machines.org/software.html`
- Some implementations (such as `LIBSVM`) can handle multi-class classification
- `SVMLight` is one of the earliest and most frequently used implementations of SVMs
- Several `Matlab` toolboxes for SVMs are available

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