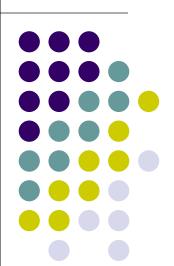
IT/PC/B/T/411

Machine Learning

Support Vector Machines and its Applications



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Overview

- Artificial Neural Networks vs. SVM
- Intro. to Support Vector Machines (SVM)
- Properties of SVM
- Applications
 - Text Categorization
- References

ANN vs SVM

- The development of ANNs followed a heuristic path, with applications and extensive experimentation preceding theory.
- In contrast, the development of SVMs involved sound theory first, then implementation and experiments.
- A significant advantage of SVMs is that whilst ANNs can suffer from multiple local minima, the solution to an SVM is global and unique.
- Two more advantages of SVMs are that that have a simple geometric interpretation and give a sparse solution.
- Unlike ANNs, the computational complexity of SVMs does not depend on the dimensionality of the input space.
- The reason that SVMs often outperform ANNs in practice is that they deal with the biggest problem with ANNs, SVMs are less prone to overfitting.

Researchers' Opinions

- "They differ radically from comparable approaches such as neural networks: SVM training always finds a global minimum, and their simple geometric interpretation provides fertile ground for further investigation." Burgess (1998)
- "Unlike conventional statistical and neural network methods, the SVM approach does not attempt to control model complexity by keeping the number of features small.
- "In contrast to neural networks SVMs automatically select their model size (by selecting the Support vectors)."

Rychetsky (2001)

Support Vector Machine (SVM)

- A classifier derived from statistical learning theory by Vapnik, et al. in 1992
- SVM became famous when, using images as input, it gave accuracy comparable to neuralnetwork with hand-designed features in a handwriting recognition task
- Currently, SVM is widely used in object detection & recognition, content-based image retrieval, text recognition, biometrics, speech recognition, etc.

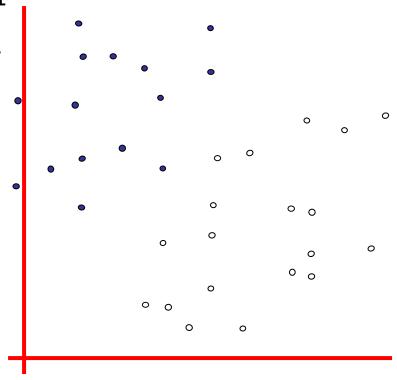


V. Vapnik

$$f(x, w, b) = sign(w, x - b)$$

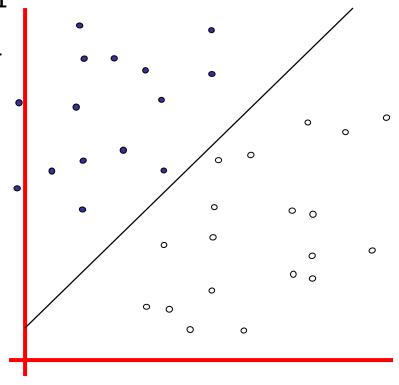
denotes +1

° denotes -1



How would you classify this data?

- f(x, w, b) = sign(w, x b)denotes +1
- ° denotes -1

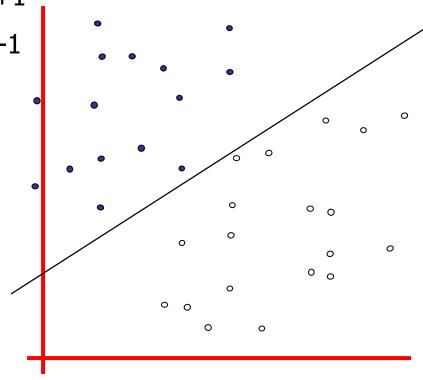


How would you classify this data?

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

• denotes +1

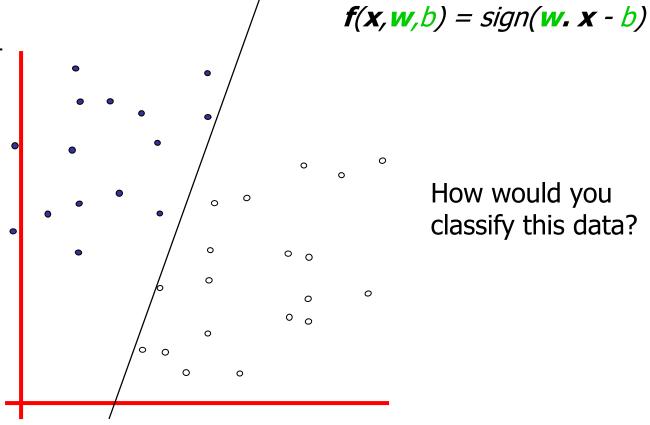
° denotes -1



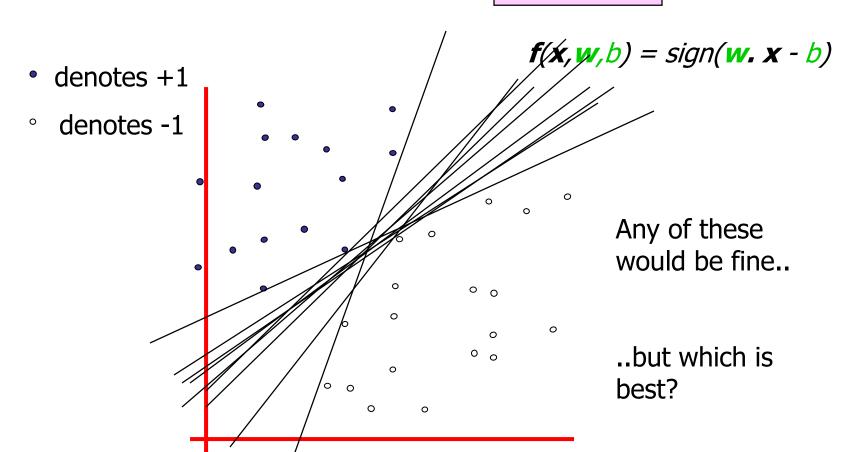
How would you classify this data?

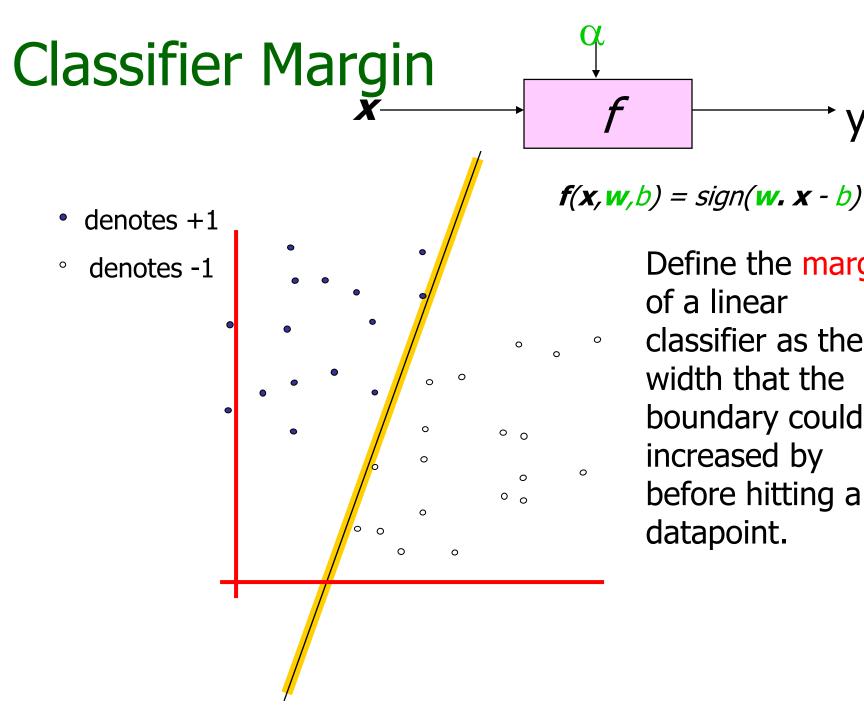
Linear Classifiers

- denotes +1
- denotes -1

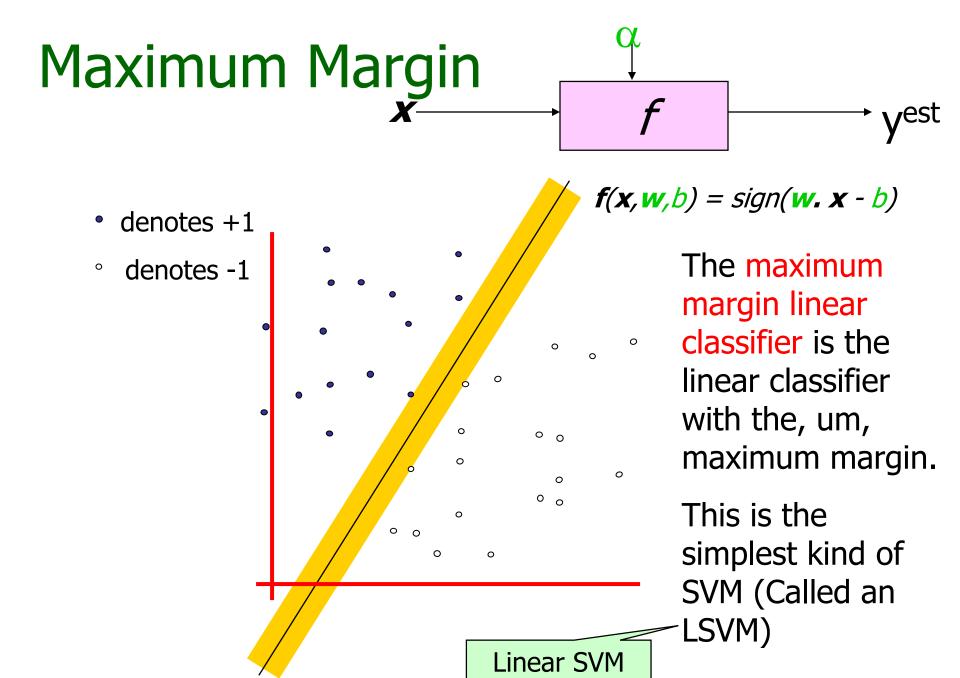


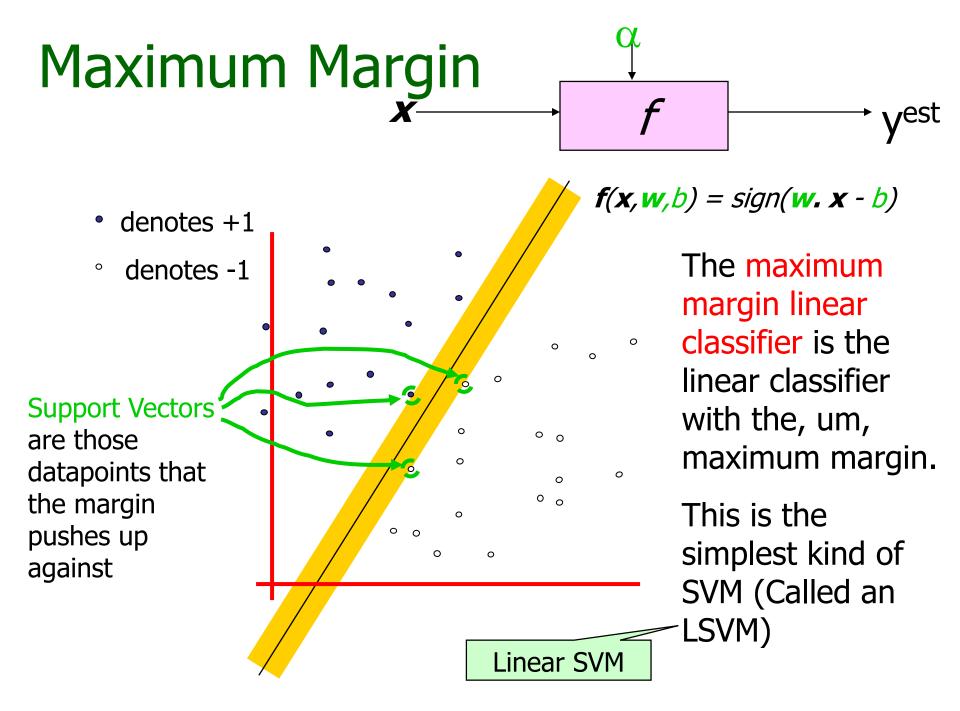
How would you classify this data?



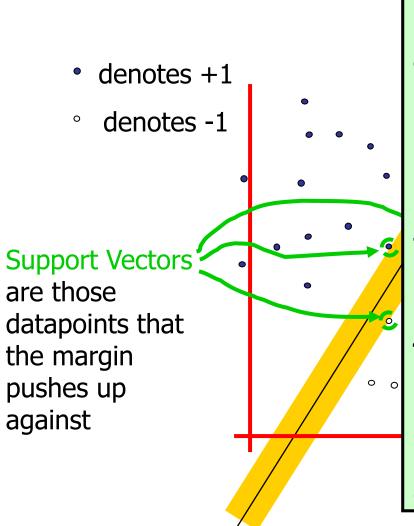


Define the margin of a linear classifier as the width that the boundary could be increased by before hitting a datapoint.



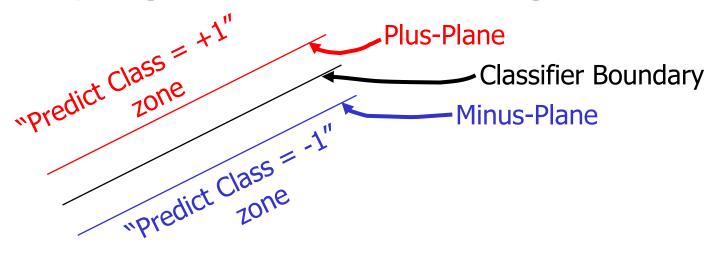


Why Maximum Margin?



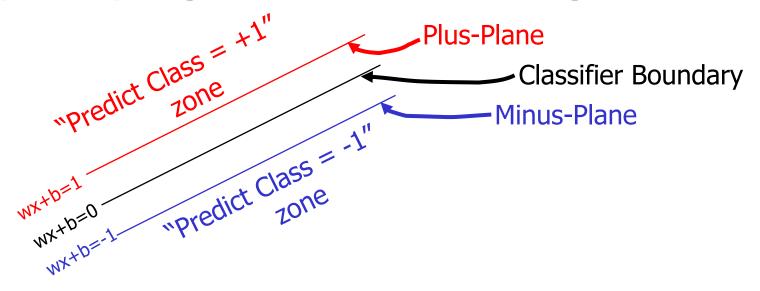
- Intuitively this feels safest.
- 2. If we've made a small error in the location of the boundary (it's been jolted in its perpendicular direction) this gives us least chance of causing a misclassification.
- 3. LOOCV is easy since the model is immune to removal of any non-support-vector datapoints.
- 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 = \{ x : w . x + b = +1 \}
```

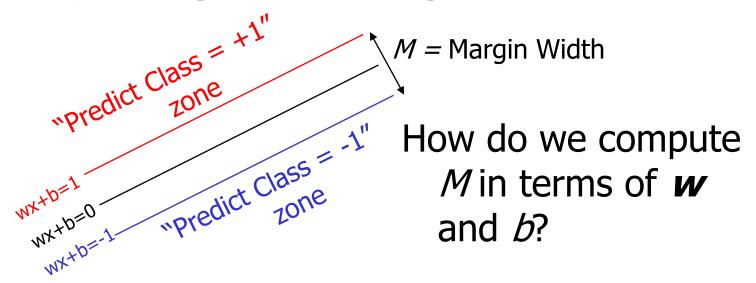
• Minus-plane =
$$\{ x : w . x + b = -1 \}$$

Classify as.. +1 if
$$w \cdot x + b >= 1$$

-1 if $w \cdot x + b <= -1$
Universe if $-1 < w \cdot x + b < 1$
explodes

- Plus-plane = $\{ x : w . x + b = +1 \}$
- Minus-plane = $\{ x : w . x + b = -1 \}$

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

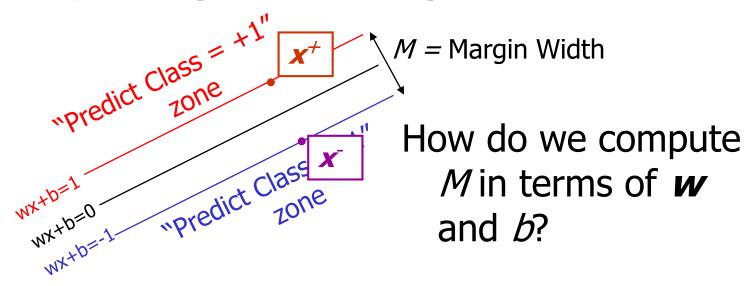


- Plus-plane = $\{ x : w . x + b = +1 \}$
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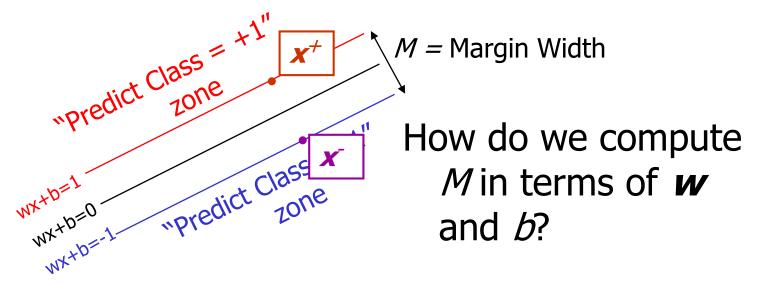
Let \mathbf{u} and \mathbf{v} be two vectors on the Plus Plane. What is $\mathbf{w} \cdot (\mathbf{u} - \mathbf{v})$?

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

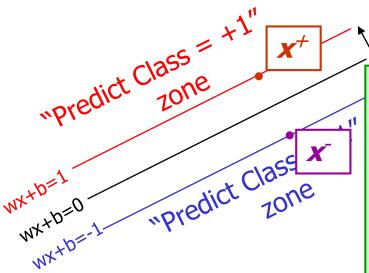


- Plus-plane = $\{ x : w . x + b = +1 \}$
- Minus-plane = $\{ x : w . x + b = -1 \}$
- The vector w is perpendicular to the Plus Plane
- Let x be any point on the minus plane
- Let x⁺ be the closest plus-plane-point to x.

Any location in R^m: not necessarily a datapoint



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

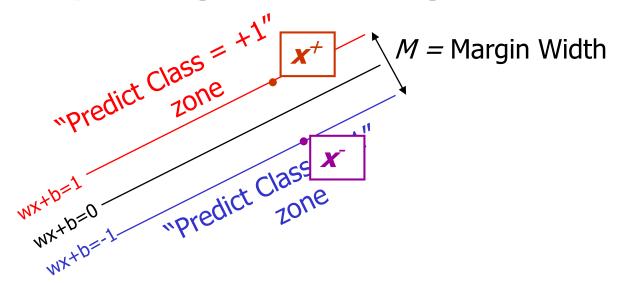


M = Margin Width

The line from **x** to **x**⁺ is perpendicular to the planes.

So to get from **x** to **x**^t travel some distance in direction **w**.

- Plus-plane = $\{x: w. x + b\}$
- Minus-plane = $\{ x : w \cdot x + b = -1 \}$
- The vector w is perpendicular to the Plus Plane
- Let x be any point on the minus plane
- Let x⁺ be the closest plus-plane-point to x.
- Claim: $\mathbf{x}^+ = \mathbf{x}^- + \lambda \mathbf{w}$ for some value of λ . Why?



What we know:

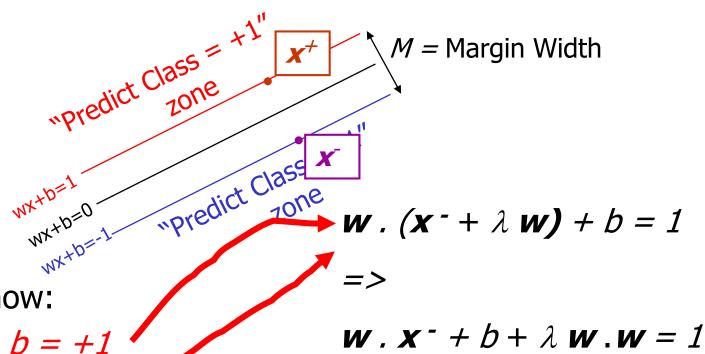
•
$$w \cdot x^+ + b = +1$$

•
$$w \cdot x + b = -1$$

•
$$\mathbf{X}^+ = \mathbf{X}^- + \lambda \mathbf{W}$$

•
$$|x^+ - x^-| = M$$

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



What we know:

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$$w \cdot x^+ + b = +1$$

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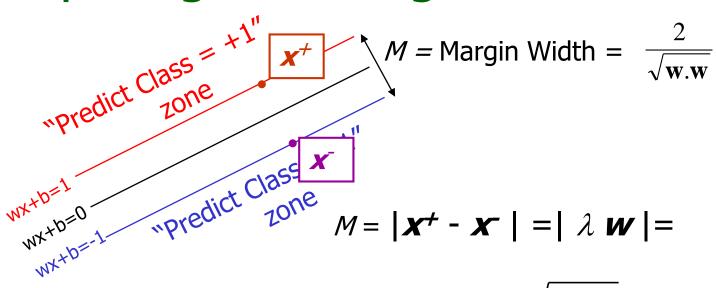
It's now easy to get *M* in terms of *w* and *b*

$$=>$$

$$-1 + \lambda w.w = 1$$

$$=>$$

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



What we know:

•
$$w \cdot x^+ + b = +1$$

•
$$w \cdot x + b = -1$$

•
$$\mathbf{X}^+ = \mathbf{X}^- + \lambda \mathbf{W}$$

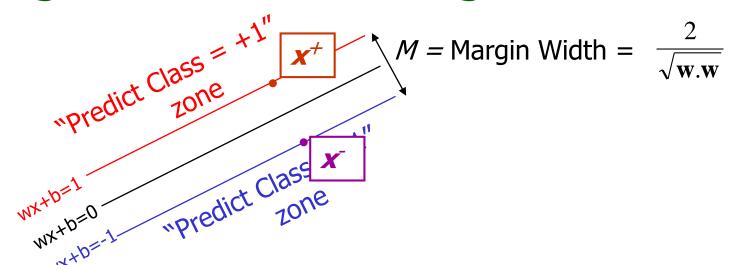
•
$$|x^+ - x^-| = M$$

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

$$=\lambda \mid \mathbf{w} \mid = \lambda \sqrt{\mathbf{w}.\mathbf{w}}$$

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

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 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
$$\underset{\mathbf{u}}{\operatorname{arg\,max}} c + \mathbf{d}^T \mathbf{u} + \frac{\mathbf{u}^T R \mathbf{u}}{2}$$
 Quadratic criterion

$$a_{11}u_1 + a_{12}u_2 + ... + a_{1m}u_m \le b_1$$

$$a_{21}u_1 + a_{22}u_2 + ... + a_{2m}u_m \le b_2$$

$$\vdots$$

$$a_{n1}u_1 + a_{n2}u_2 + ... + a_{nm}u_m \le b_n$$

$$n \text{ additional linear inequality constraints}$$

$$a_{n1}u_1 + a_{n2}u_2 + ... + a_{nm}u_m \le b_n$$

constraints

And subject to

$$a_{n1}u_{1} + a_{n2}u_{2} + \dots + a_{nm}u_{m} \leq b_{n}$$

$$a_{(n+1)1}u_{1} + a_{(n+1)2}u_{2} + \dots + a_{(n+1)m}u_{m} = b_{(n+1)}$$

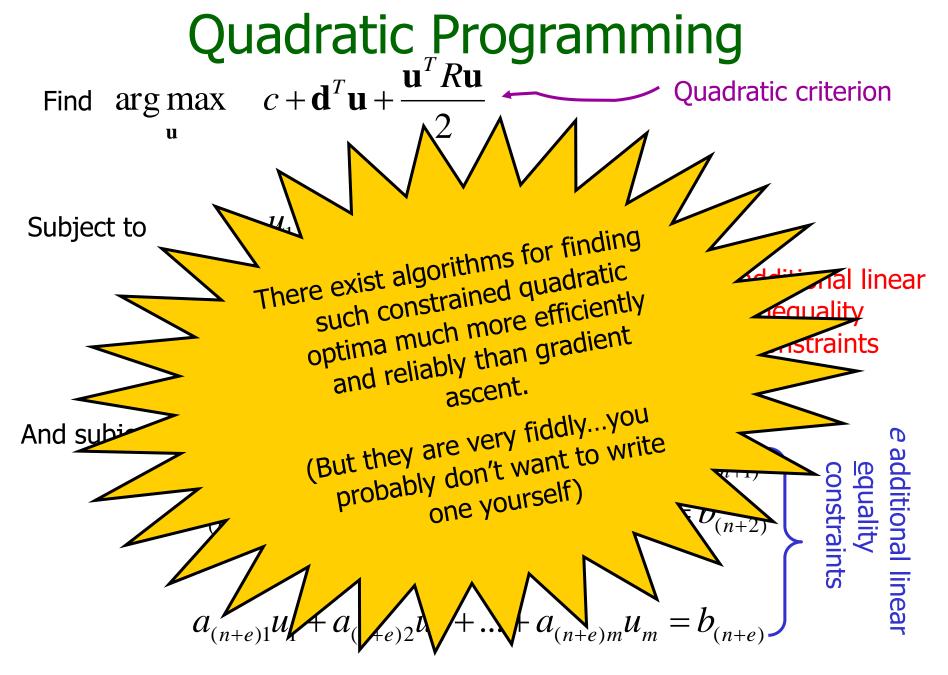
$$a_{(n+2)1}u_{1} + a_{(n+2)2}u_{2} + \dots + a_{(n+2)m}u_{m} = b_{(n+2)}$$

$$\vdots$$

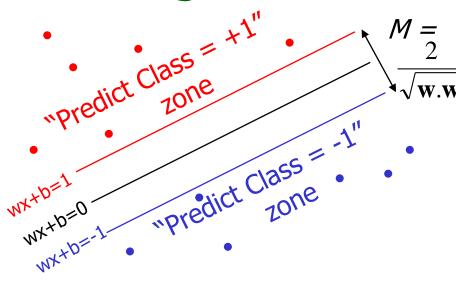
$$a_{(n+e)1}u_{1} + a_{(n+e)2}u_{2} + \dots + a_{(n+e)m}u_{m} = b_{(n+e)}$$

$$\vdots$$

$$a_{(n+e)1}u_{1} + a_{(n+e)2}u_{2} + \dots + a_{(n+e)m}u_{m} = b_{(n+e)}$$



Learning the Maximum Margin Classifier



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

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

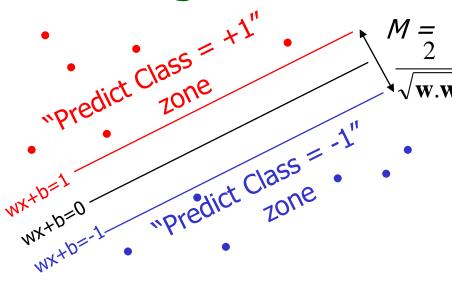
Assume *R* datapoints, each $(\mathbf{x}_k, \mathbf{y}_k)$ where $\mathbf{y}_k = +/-1$

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 \boldsymbol{w} , \boldsymbol{b} we can

- Compute whether all data points are in the correct half-planes
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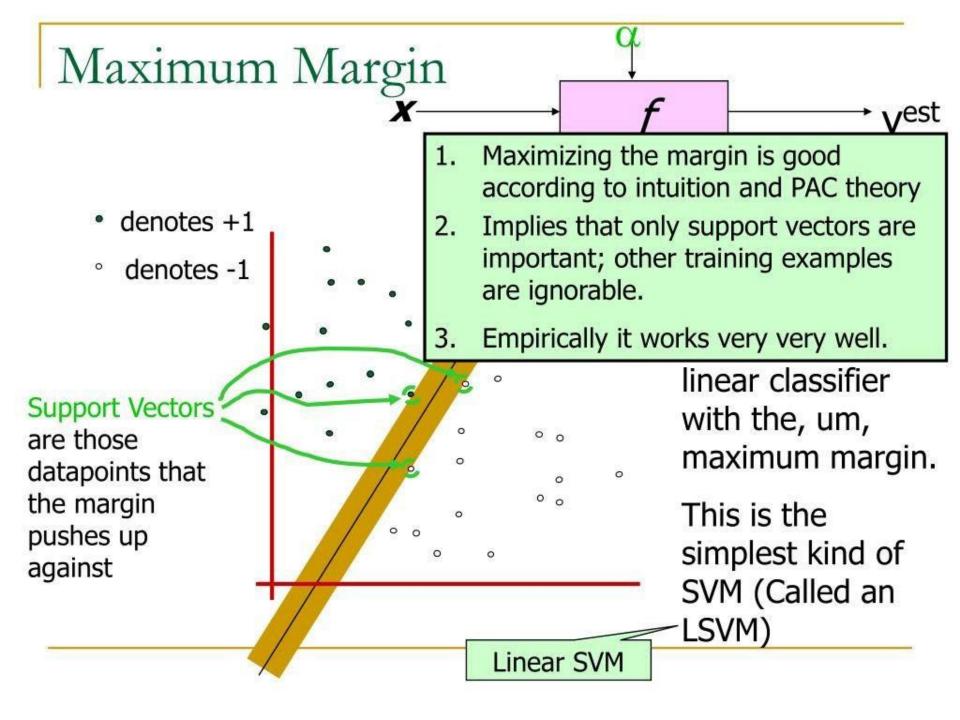
What should our quadratic optimization criterion be?

Minimize www

How many constraints will we have? *R*

What should they be?

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

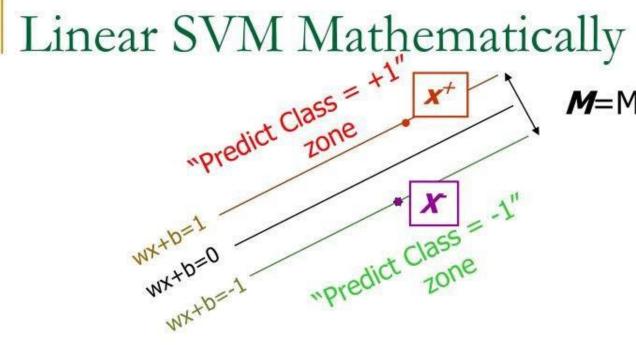


Let me digress to...what is PAC Theory?

- Two important aspects of complexity in machine learning.
- First, sample complexity: in many learning problems, training data is expensive and we should hope not to need too much of it.
- Secondly, computational complexity: A neural network, for example, which takes an hour to train may be of no practical use in complex financial prediction problems.
- Important that both the amount of training data required for a prescribed level of performance and the running time of the learning algorithm in learning from this data do not increase too dramatically as the `difficulty' of the learning problem increases.

Let me digress to...what is PAC Theory?

- Such issues have been formalised and investigated over the past decade within the field of `computational learning theory'.
- One popular framework for discussing such problems is the probabilistic framework which has become known as the 'probably approximately correct', or PAC, model of learning.



M=Margin Width

What we know:

$$\mathbf{w} \cdot \mathbf{X}^+ + b = +1$$

$$w \cdot x + b = -1$$

$$\mathbf{w} \cdot (\mathbf{x}^+ - \mathbf{x}^-) = 2$$

$$M = \frac{(x^+ - x^-) \cdot w}{|w|} = \frac{2}{|w|}$$

Linear SVM Mathematically

Goal: 1) Correctly classify all training data

$$wx_i + b \ge 1 \qquad \text{if } y_i = +1 \\ wx_i + b \le 1 \qquad \text{if } y_i = -1 \\ y_i(wx_i + b) \ge 1 \qquad \text{for all i } 2$$
2) Maximize the Margin same as minimize
$$\frac{M}{2} = \frac{2}{|w|}$$

We can formulate a Quadratic Optimization Problem and solve for w and b

Minimize
$$\Phi(w) = \frac{1}{2} w^t w$$

subject to $y_i(wx_i + b) \ge 1$ $\forall i$

Solving the Optimization Problem

```
Find w and b such that \Phi(\mathbf{w}) = \frac{1}{2} \mathbf{w}^{\mathrm{T}} \mathbf{w} is minimized; and for all \{(\mathbf{x_i}, y_i)\}: y_i (\mathbf{w}^{\mathrm{T}} \mathbf{x_i} + b) \ge 1
```

- Need to optimize a quadratic function subject to linear constraints.
- Quadratic optimization problems are a well-known class of mathematical programming problems, and many (rather intricate) algorithms exist for solving them.
- The solution involves constructing a dual problem where a Lagrange multiplier α_i is associated with every constraint in the primary problem:

```
Find \alpha_1...\alpha_N such that \mathbf{Q}(\mathbf{\alpha}) = \sum \alpha_i - \frac{1}{2} \sum \sum \alpha_i \alpha_j y_i y_j \mathbf{x_i}^T \mathbf{x_j} \text{ is maximized and}
(1) \sum \alpha_i y_i = 0
(2) \alpha_i \ge 0 for all \alpha_i
```

A digression... Lagrange Multipliers

- In mathematical optimization, the method of Lagrange multipliers provides a strategy for finding the maxima and minima of a function subject to constraints.
- For instance, consider the optimization problem maximize f(x,y) subject to g(x,y)=c.
- We introduce a new variable (λ) called a Lagrange multiplier, and study the Lagrange function defined by $\Lambda(x,y,\lambda) = f(x,y) + \lambda \cdot \left(g(x,y) c\right).$ (the λ term may be either added or subtracted.)
- If (x,y) is a maximum for the original constrained problem, then there exists a λ such that (x,y,λ) is a stationary point for the Lagrange function
- (stationary points are those points where the partial derivatives of Λ are zero).

The Optimization Problem Solution

The solution has the form:

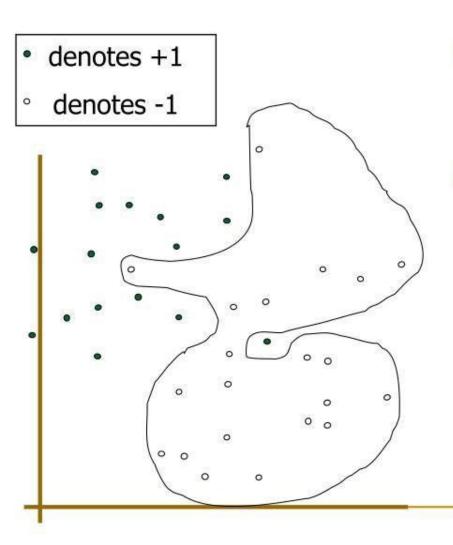
$$\mathbf{w} = \sum \alpha_i y_i \mathbf{x_i}$$
 $b = y_k - \mathbf{w^T} \mathbf{x_k}$ for any $\mathbf{x_k}$ such that $\alpha_k \neq 0$

- Each non-zero α_i indicates that corresponding x_i is a support vector.
- Then the classifying function will have the form:

$$f(\mathbf{x}) = \sum \alpha_i y_i \mathbf{x_i}^{\mathsf{T}} \mathbf{x} + b$$

- Notice that it relies on an inner product between the test point x and the support vectors x_i – we will return to this later.
- Also keep in mind that solving the optimization problem involved computing the inner products x_i^Tx_j between all pairs of training points.

Dataset with noise

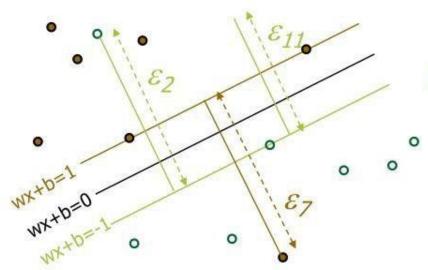


- Hard Margin: So far we require all data points be classified correctly
 - No training error
- What if the training set is noisy?
 - Solution 1: use very powerful kernels

OVERFITTING!

Soft Margin Classification

Slack variables ξi can be added to allow misclassification of difficult or noisy examples.



What should our quadratic optimization criterion be?

Minimize

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

Hard Margin v.s. Soft Margin

The old formulation:

```
Find w and b such that  \Phi(\mathbf{w}) = \frac{1}{2} \mathbf{w}^{\mathrm{T}} \mathbf{w}  is minimized and for all \{(\mathbf{x_i}, y_i)\}   y_i (\mathbf{w}^{\mathrm{T}} \mathbf{x_i} + \mathbf{b}) \ge 1
```

The new formulation incorporating slack variables:

```
Find w and b such that  \Phi(\mathbf{w}) = \frac{1}{2} \mathbf{w}^{\mathrm{T}} \mathbf{w} + C \Sigma \xi_{i}  is minimized and for all \{(\mathbf{x_i}, y_i)\}  y_i (\mathbf{w}^{\mathrm{T}} \mathbf{x_i} + b) \ge 1 - \xi_i  and \xi_i \ge 0 for all i
```

Parameter C can be viewed as a way to control overfitting.

Linear SVMs: Overview

- The classifier is a separating hyperplane.
- Most "important" training points are support vectors; they define the hyperplane.
- Quadratic optimization algorithms can identify which training points x_i are support vectors with non-zero Lagrangian multipliers α_j.
- Both in the dual formulation of the problem and in the solution training points appear only inside dot products:

Find $\alpha_1 ... \alpha_N$ such that

 $Q(\alpha) = \sum \alpha_i - \frac{1}{2} \sum \sum \alpha_i \alpha_i y_i y_j x_i^T x_j$ is maximized and

- (1) $\Sigma \alpha_i y_i = 0$
- (2) $0 \le \alpha_i \le C$ for all α_i

$$f(\mathbf{x}) = \sum \alpha_i y_i \mathbf{x}_i^{\mathrm{T}} \mathbf{x} + b$$

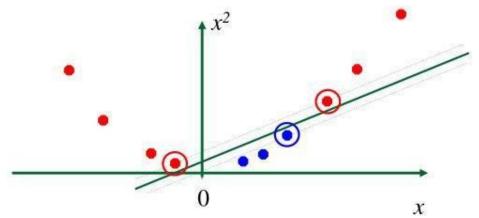
Non-linear SVMs

Datasets that are linearly separable with some noise work out great:

But what are we going to do if the dataset is just too hard?

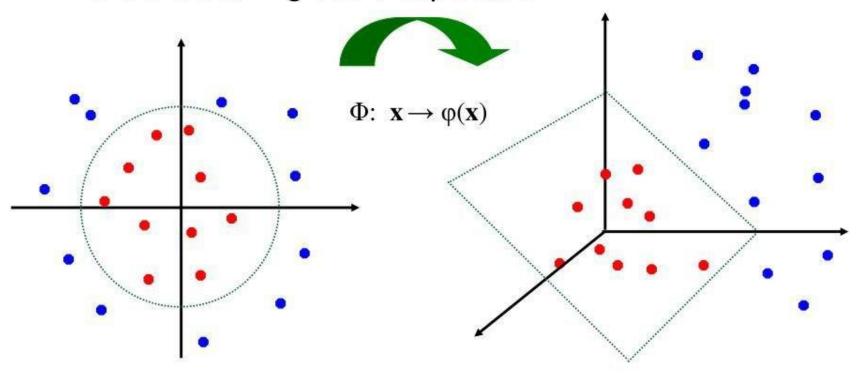


How about... mapping data to a higher-dimensional space:



Non-linear SVMs: Feature spaces

General idea: the original input space can always be mapped to some higher-dimensional feature space where the training set is separable:



The "Kernel Trick"

- The linear classifier relies on dot product between vectors $K(x_i,x_j)=x_i^Tx_j$
- If every data point is mapped into high-dimensional space via some transformation Φ: $x \to φ(x)$, the dot product becomes:

$$K(\mathbf{x}_i, \mathbf{x}_j) = \varphi(\mathbf{x}_i)^T \varphi(\mathbf{x}_j)$$

- A kernel function is some function that corresponds to an inner product in some expanded feature space.
- Example:

2-dimensional vectors $\mathbf{x} = [x_1 \ x_2]$; let $K(\mathbf{x}_i, \mathbf{x}_j) = (1 + \mathbf{x}_i^T \mathbf{x}_j)^2$, Need to show that $K(\mathbf{x}_i, \mathbf{x}_j) = \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j)$:

$$K(\mathbf{x_i}, \mathbf{x_j}) = (1 + \mathbf{x_i}^{\mathrm{T}} \mathbf{x_j})^2,$$

$$= 1 + x_{i1}^2 x_{j1}^2 + 2 x_{i1} x_{j1} x_{i2} x_{j2} + x_{i2}^2 x_{j2}^2 + 2 x_{i1} x_{j1} + 2 x_{i2} x_{j2}$$

$$= [1 \ x_{i1}^2 \ \sqrt{2} \ x_{i1} x_{i2} \ x_{i2}^2 \ \sqrt{2} x_{i1} \ \sqrt{2} x_{i2}]^{\mathrm{T}} [1 \ x_{j1}^2 \ \sqrt{2} \ x_{j1} x_{j2} \ x_{j2}^2 \ \sqrt{2} x_{j1} \ \sqrt{2} x_{j2}]$$

$$= \varphi(\mathbf{x_i})^{\mathrm{T}} \varphi(\mathbf{x_j}), \quad \text{where } \varphi(\mathbf{x}) = [1 \ x_{1}^2 \ \sqrt{2} \ x_{1} x_{2} \ x_{2}^2 \ \sqrt{2} x_{1} \ \sqrt{2} x_{2}]$$

What Functions are Kernels?

- For some functions $K(\mathbf{x_i}, \mathbf{x_j})$ checking that $K(\mathbf{x_i}, \mathbf{x_i}) = \phi(\mathbf{x_i})^{\mathrm{T}} \phi(\mathbf{x_i}) \text{ can be cumbersome.}$
- Mercer's theorem:

Every semi-positive definite symmetric function is a kernel

Examples of Kernel Functions

- Linear: K(x_i,x_j)= x_i^Tx_j
- Polynomial of power p: K(x_i,x_j)= (1+ x_i^Tx_j)^p
- Gaussian (radial-basis function network):

$$K(\mathbf{x_i}, \mathbf{x_j}) = \exp(-\frac{\left\|\mathbf{x_i} - \mathbf{x_j}\right\|^2}{2\sigma^2})$$

Sigmoid: $K(\mathbf{x_i}, \mathbf{x_i}) = \tanh(\beta_0 \mathbf{x_i}^T \mathbf{x_i} + \beta_1)$

Non-linear SVMs Mathematically

Dual problem formulation:

Find $\alpha_1 ... \alpha_N$ such that

$$Q(\alpha) = \sum \alpha_i - \frac{1}{2} \sum \alpha_i \alpha_i y_i y_j K(x_i, x_j)$$
 is maximized and

- (1) $\Sigma \alpha_i y_i = 0$
- (2) $\alpha_i \ge 0$ for all α_i

The solution is:

$$f(\mathbf{x}) = \sum \alpha_i y_i K(\mathbf{x}_i, \mathbf{x}_j) + b$$

• Optimization techniques for finding α_i 's remain the same!

Nonlinear SVM - Overview

- SVM locates a separating hyperplane in the feature space and classify points in that space
- It does not need to represent the space explicitly, simply by defining a kernel function
- The kernel function plays the role of the dot product in the feature space.

Properties of SVM

- Flexibility in choosing a similarity function
- Sparseness of solution when dealing with large data sets
 - only support vectors are used to specify the separating hyperplane
- Ability to handle large feature spaces
 - complexity does not depend on the dimensionality of the feature space
- Overfitting can be controlled by soft margin approach
- Nice math property: a simple convex optimization problem which is guaranteed to converge to a single global solution
- Feature Selection

SVM Applications

- SVM has been used successfully in many real-world problems
 - text (and hypertext) categorization
 - image classification different types of subproblems
 - bioinformatics (Protein classification, Cancer classification)
 - hand-written character recognition

Weakness of SVM

- It is sensitive to noise
 - A relatively small number of mislabeled examples can dramatically decrease the performance
- It only considers two classes
 - how to do multi-class classification with SVM?
 - Answer:
 - 1) with output arity m, learn m SVM's
 - SVM 1 learns "Output==1" vs "Output != 1"
 - SVM 2 learns "Output==2" vs "Output != 2"
 - o :
 - SVM m learns "Output==m" vs "Output != m"
 - 2)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.

Application: Text Categorization

- Task: The classification of natural text (or hypertext) documents into a fixed number of predefined categories based on their content.
 - email filtering, web searching, sorting documents by topic, etc..
- A document can be assigned to more than one category, so this can be viewed as a series of binary classification problems, one for each category

Application: Face Expression Recognition

- Construct feature space, by use of eigenvectors or other means
- Multiple class problem, several expressions
- Use multi-class SVM

Some Issues

Choice of kernel

- Gaussian or polynomial kernel is default
- if ineffective, more elaborate kernels are needed

Choice of kernel parameters

- e.g. σ in Gaussian kernel
- σ is the distance between closest points with different classifications
- In the absence of reliable criteria, applications rely on the use of a validation set or cross-validation to set such parameters.
- Optimization criterion Hard margin v.s. Soft margin
 - a lengthy series of experiments in which various parameters are tested

Additional Resources

LibSVM

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.

The VC/SRM/SVM Bible:

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

http://www.kernel-machines.org/

Reference

- Support Vector Machine Classification of Microarray Gene Expression Data, Michael P. S. Brown William Noble Grundy, David Lin, Nello Cristianini, Charles Sugnet, Manuel Ares, Jr., David Haussler
- www.cs.utexas.edu/users/mooney/cs391L/svm.ppt
- Text categorization with Support Vector Machines: learning with many relevant features
 - T. Joachims, ECML 98