













Inspire...Educate...Transform.

# **Predictive Analytics**

**SVM** 

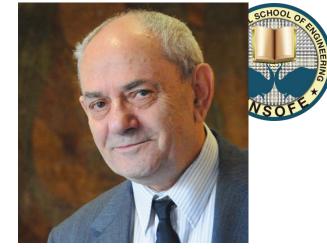
Dr. Suryaprakash Kompalli Senior Mentor, INSOFE



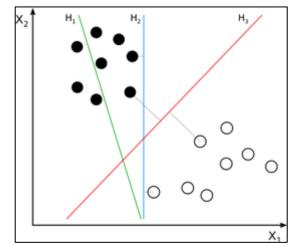
### **SUPPORT VECTOR MACHINES**

#### **SVM** – Curtain Raiser

- Support Vector Machines is arguably the most important & interesting recent discovery in Machine Learning.
- SVMs have a clever way to prevent over-fitting
- SVMs have a very clever way to use a huge number of features without requiring nearly as much computation as seems to be necessary.



Vladimir Vapnik Invented SVM in 1963!!! Non-linear classifier in 1992!!!



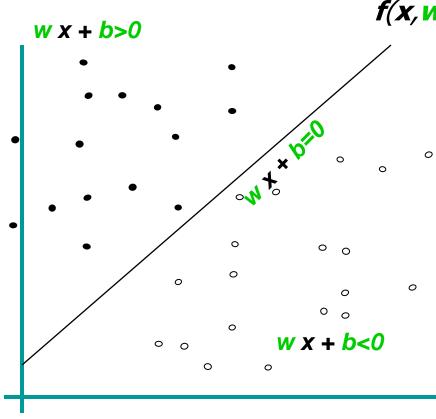
 $\rm H_1$  does not separate the classes.  $\rm H_2$  does, but only with a small margin.  $\rm H_3$  separates them with the maximum margin.  $\rm source:$ 

https://en.wikipedia.org/wiki/Support\_vector\_machine



•denotes +1

°denotes -1



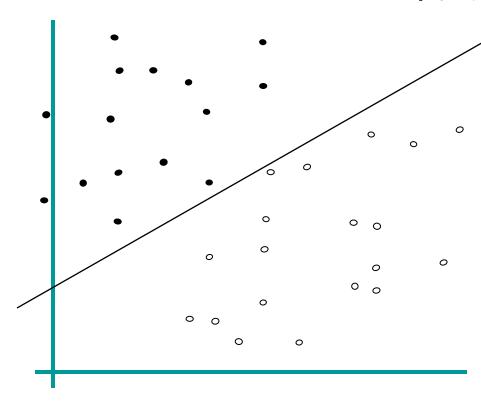
f(x, w, b) = sign(w x + b)

How would you classify this data?

Is a single line the only solution?



- denotes +1
- ° denotes -1

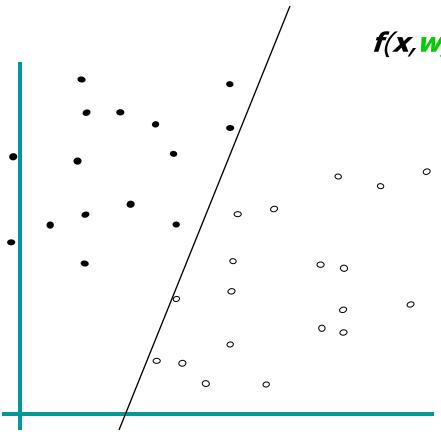


f(x, w, b) = sign(w x + b)

How would you classify this data?

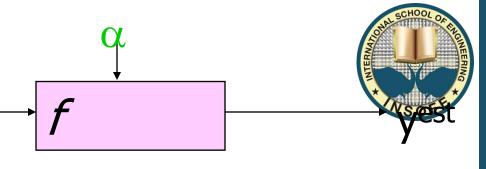


- denotes +1
- ° denotes -1



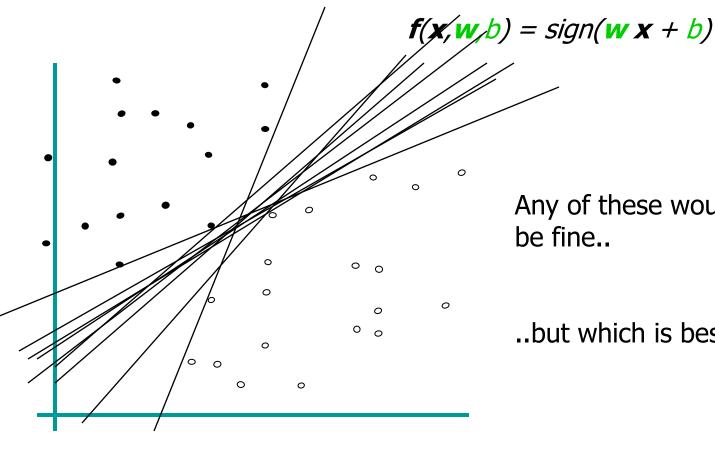
f(x, w, b) = sign(w x + b)

How would you classify this data?



denotes +1

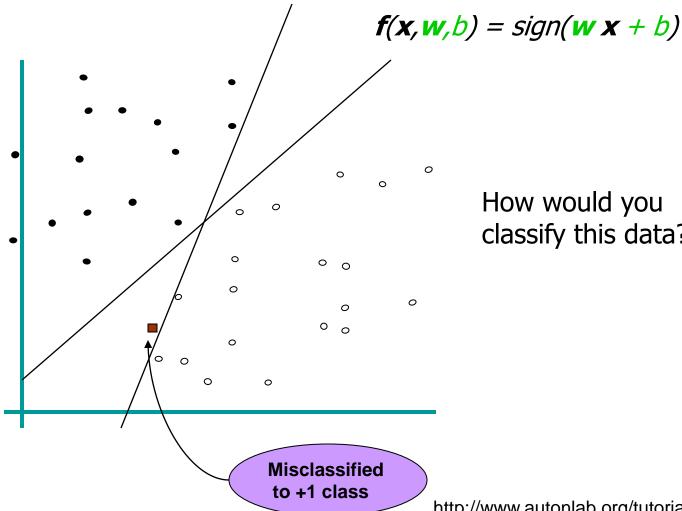
denotes -1



Any of these would be fine...

..but which is best?

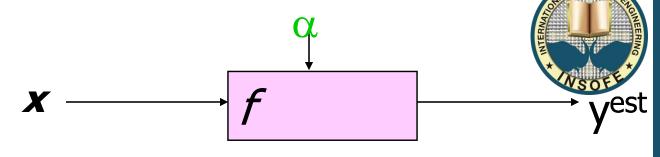
- denotes +1
- denotes -1



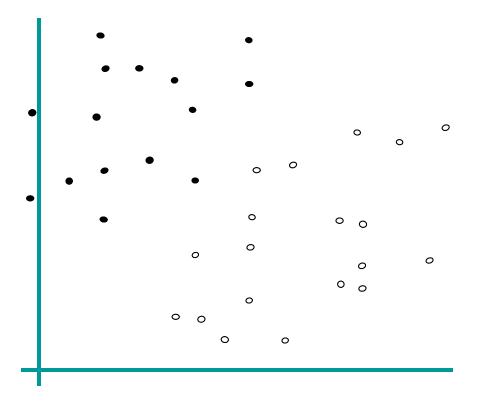
How would you classify this data?

http://www.autonlab.org/tutorials/svm15.pdf

# Classifier Margin



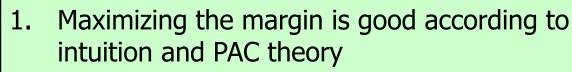
- denotes +1
- denotes -1



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 datapoint.

# Maximum Margin



- 2. Implies that only support vectors are important; other training examples are ignorable.
- 3. Empirically it works very very well.

denotes +1

° denotes -1

#### **Support Vectors**

are those datapoints that the margin pushes up against

classifier with the, um, maximum margin.

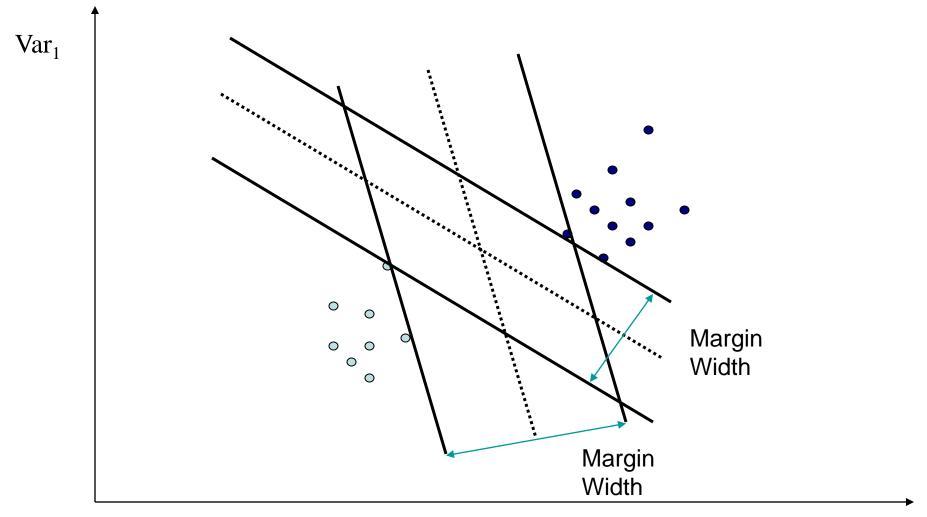
This is the simplest kind of SVM (Called an LSVM)

Linear SVM

0

# **Maximizing the Margin**





Var<sub>2</sub>

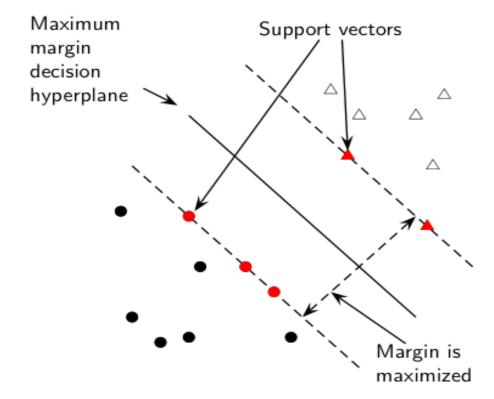
# Why maximize the margin?



Points near decision surface → uncertain classification decisions (50% either way).

A classifier with a large margin makes no low certainty classification decisions.

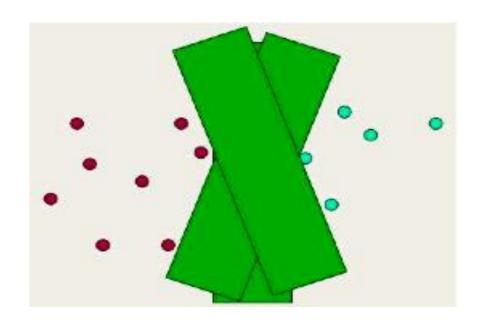
Gives classification safety margin w.r.t slight errors in measurement



# Why maximize the margin?

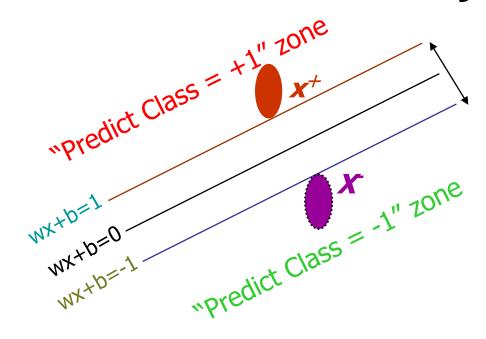


- SVM classifier: large margin around decision boundary
- Compare to decision hyperplane: place fat separator between classes
- Fewer choices of where it can be put
  - Decreased memory capacity
  - Increased ability to correctly generalize to test data





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



$$M = |x^+-x^-|$$

Let us express the planes as:

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

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

From above two equations:

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

If U and V are vectors on x+ plane

**w** . **U** + 
$$b = +1$$

$$w \cdot V + b = +1$$

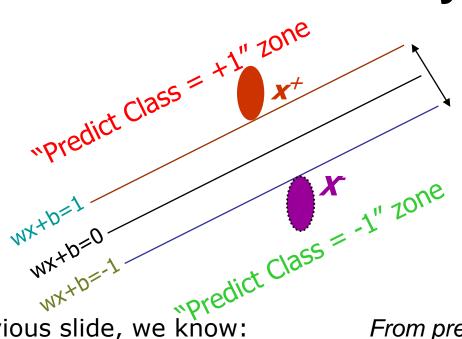
w . (*U-V*) = 0, hence w is perpendicular to  $x^+$  and x are parallel to each other

From above two observations, we can say:

$$\mathbf{X}^+ = \mathbf{X}^- + k \mathbf{W}$$

http://www.cs.cmu.edu/~awm/tutorials





**M**=Margin Width

$$M = |x^+-x^-|$$

From previous slide, we know:

$$\mathbf{W} \cdot (\mathbf{x}^{+} - \mathbf{x}^{-}) = 2$$
  
 $\mathbf{W}^{-1} \cdot \mathbf{W} \cdot (\mathbf{x}^{+} - \mathbf{x}^{-}) = \mathbf{W}^{-1} \cdot 2$   
 $(\mathbf{x}^{+} - \mathbf{x}^{-}) = \mathbf{W}^{-1} \cdot 2 \dots Eq 1$ 

From Eq 1 and Eq 2:

$$w^{-1} \cdot 2 = k w$$
  
 $k = \frac{w^{-1} \cdot 2}{w} = \frac{2}{w \cdot w} \dots \text{Eq } 3$ 

From previous slide, we know:

$$x^{+} = x^{-} + k w$$
  
 $x^{+} - x = k w ... Eq 2$ 

Margin, 
$$M = |x^+-x^-| = |kw| = k/w | = k\sqrt{w \cdot w}$$

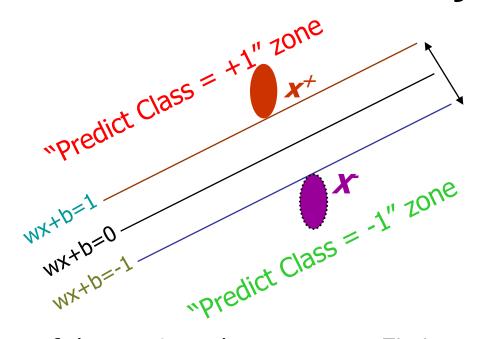
Substituting k from Eq 3 we have:

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

http://www.cs.cmu.edu/~awm/tutorials

http://www.autonlab.org/tutorials/svm15.pdf





**M**=Margin Width

$$M = |x^+-x^-|$$

Given a set of data points that satisfy:

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

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

Find a value of "w" and "b" such that:

$$M = \frac{2}{\sqrt{w \cdot w}}$$
 is maximized

Above is the same as:

$$\frac{1}{2}\sqrt{w.w}$$
 is minimized





Goal: 1) Correctly classify all training data

$$wx_{i} + b \ge 1$$

$$wx_{i} + b \le -1$$

$$y_{i}(wx_{i} + b) \ge 1$$

$$y_{i}(w.x_{i} + b) - 1 \ge 0 \text{ for all i}$$

$$\frac{1}{2}\sqrt{w.w}$$

#### 2) Minimize

This is a Quadratic Optimization Problem in linear constraints. Solve for w & b.



Goal: 1) Correctly classify all training data

$$w. x_i + b \ge 1 \text{ if } y_i = +1$$
  
 $w. x_i + b \le -1 \text{ if } y_i = -1$   
 $y_i(w. x_i + b) - 1 \ge 0 \text{ for all i}$ 

2) Minimize 
$$\frac{1}{2}\sqrt{w.w}$$

This is a Quadratic Optimization Problem in linear constraints. Solve for w & b.

# Linear (hard-margin) SVM - formulation



• Find w,b that solves

$$\min \frac{1}{2} \|w\|^2$$
s.t.  $y_i(w \cdot x_i + b) \ge 1, \ \forall x_i$ 

- Problem is convex so, there is a unique global minimum value (when feasible)
- Non-solvable if the data is not linearly separable
- Quadratic Programming
  - Very efficient computationally with modern constraint optimization engines (handles thousands of constraints and training instances).

# Solving the Optimization Problem



Find w, b such that:

Minimize 
$$f(x)$$
:  $1/2 ||w||^2$   
Subject to:  $g(x)$ :  $y_i(w, x_i + b) - 1 = 0$ 

The solution involves constructing a *dual problem* where a *Lagrange* multiplier  $\alpha_i$  is associated with every constraint in the primary problem:

Find  $\alpha_{I}...\alpha_{N}$  such that  $L_{D} = -\frac{1}{2}\sum_{i=0}^{n}\alpha_{i}\alpha_{j}y_{i}y_{j}(x_{i}.x_{j}) + \sum_{i=0}^{n}\alpha_{i} \text{ is Maximized}$   $Subject \ to: \sum_{i=0}^{n}\alpha_{i}y_{i} = 0, \alpha_{i} > 0$ 

*Once we find*  $\alpha_1...\alpha_N$ 

Solution 
$$w = \sum_{i=0}^{n} a_i y_i x_i$$

#### **Derivations**

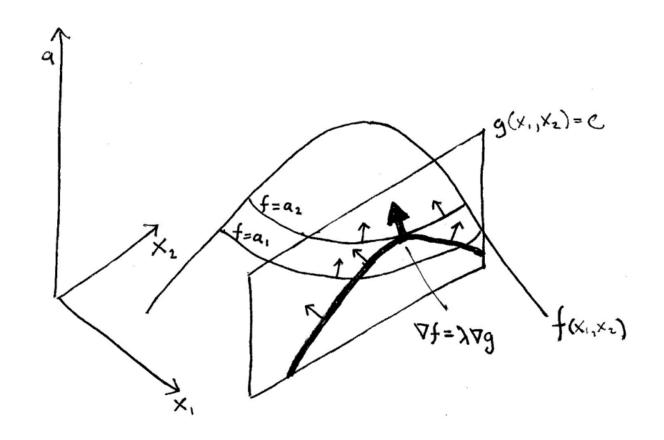


 The next 7 slides are only for reference to understand derivation details !!!



## **Optimization with Lagrange Multipliers**





http://tutorial.math.lamar.edu/Classes/CalcIII/LagrangeMultipliers.aspx http://www.slimy.com/~steuard/teaching/tutorials/Lagrange.html

## **Lagrange Multipliers**



- Minimize  $U=x^2 + y^2$
- Subject to  $g = x^2+y^2+2x-2y+1 = 0$

Lagrange equation

•  $L=U-\lambda g=0$ 



## **Method of Lagrange multipliers**

$$U=x^{2} + y^{2}$$

$$g= x^{2}+y^{2}+2x-2y+1=0$$

• 
$$\frac{\partial L}{\partial x} = 2x - \lambda(2x + 2) = 0$$
;  $x - \lambda(x + 1) = 0$ 

• 
$$\frac{\partial L}{\partial y} = 2y - \lambda(2y - 2) = 0; y - \lambda(y - 1) = 0$$

$$\bullet \frac{\partial L}{\partial \lambda} = -1(x^2 + y^2 + 2x - 2y + 1) = 0$$

 From 1 and 2, we get y=-x and substituting in 3, we get x and y values.

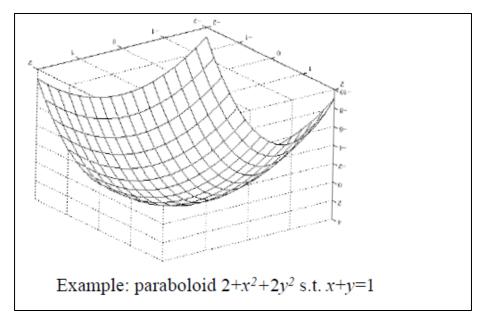


Find w and b such that

**f:** 
$$\Phi(\mathbf{w}) = \frac{1}{2} \mathbf{w}^{\mathrm{T}} \mathbf{w}$$
 is minimized and for all  $\{(\mathbf{x_i}, y_i)\}$   $g: y_i (\mathbf{w}^{\mathrm{T}} \mathbf{x_i} + \mathbf{b}) \ge 1$ 

f is a quadratic function, and a paraboloid, and is known to have unique solution.

f,g can be converted into Lagrangian form



Reference: svm-notes-long-08



Minimize 
$$f(x)$$
:  $1/2 ||w||^2$   
Subject to:  $g(x)$ :  $y_i(w.x_i + b) - 1 = 0$ 

Convert to Lagrange form:

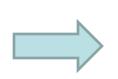
$$\min L = 1/2 ||w||^2 - \sum_{i=0}^{n} \alpha_i [y_i(w, x_i + b) - 1]$$

$$\min L = 1/2 ||w||^2 - \sum_{i=0}^{n} \alpha_i y_i(w, x_i + b) + \sum_{i=0}^{n} \alpha_i$$

Derivatives at Minima =0

$$\frac{\partial L}{\partial w}: w - \sum_{i=0}^{n} \alpha_i y_i x_i = 0$$

$$\frac{\partial L}{\partial b}: \sum_{i=0}^{n} \alpha_i y_i = 0$$



$$w = \sum_{i=0}^{n} \alpha_i y_i x_i$$
$$\sum_{i=0}^{n} \alpha_i y_i = 0$$



Minimize 
$$f(x)$$
:  $1/2 ||w||^2$   
Subject to:  $g(x)$ :  $y_i(w.x_i + b) - 1 = 0$ 

#### Convert to Lagrange form:

$$\min L = 1/2 ||w||^2 - \sum_{i=0}^{n} \alpha_i [y_i(w, x_i + b) - 1]$$

$$\min L = 1/2 ||w||^2 - \sum_{i=0}^{n} \alpha_i y_i(w, x_i + b) + \sum_{i=0}^{n} \alpha_i$$

$$\max L_D = -\frac{1}{2} \sum_{i=0}^{n} \alpha_i y_i x_i$$

$$\sum_{i=0}^{n} \alpha_i y_i = 0$$
Such that:

$$\max L_D = -\frac{1}{2} \sum_{i=0}^n \alpha_i \alpha_j y_i y_j (x_i, x_j) + \sum_{i=0}^n \alpha_i$$

$$Such that: \sum_{i=0}^n \alpha_i y_i = 0, \alpha_i > 0$$

Substitute these values to get the dual solution:



Minimize 
$$f(x)$$
:  $1/2 ||w||^2$   
Subject to:  $g(x)$ :  $y_i(w.x_i + b) - 1 = 0$ 

Convert to Lagrange form:

$$\min L = 1/2 ||w||^2 - \sum_{i=0}^{n} a_i y_i (w. x_i + b) + \sum_{i=0}^{n} a_i$$

$$Solution w = \sum_{i=0}^{n} a_i y_i x_i \qquad \sum_{i=0}^{n} a_i y_i = 0$$

$$\max L_D = -\frac{1}{2} \sum_{i=0}^n \alpha_i \alpha_j y_i y_j (x_i, x_j) + \sum_{i=0}^n \alpha_i$$

Such that: 
$$\sum_{i=0}^{n} \alpha_i y_i = 0, \alpha_i > 0$$

Why is the dual solution used?

Ans 1: Easier to compute in case of Kernel methods.

Ans 2: Kind of related to Answer 1. If you take partial derivative of  $\max L_D WRT\alpha$ , the solution will be:

$$\sum_{i=0}^{n} \alpha_i y_i = 0, \alpha_i > 0$$

The way to solve is to find different values of  $\alpha$  and see which ones will give maximum. The original solution is much worse

Reference: svm15.pdf

## Dataset with noise



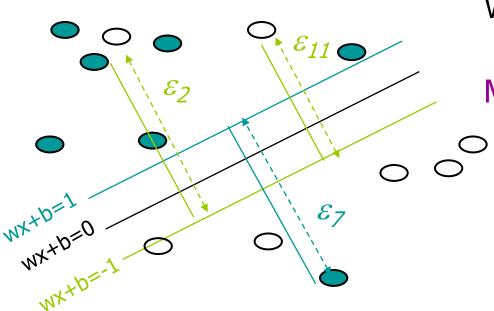
- denotes +1
- denotes -1
- Hard Margin: So far we require all data points be classified correctly
  - No training error
- What if the training set is noisy?
  - Solution 1: use very powerful kernels

#### **OVERFITTING!**

# **Soft Margin Classification**



Slack variables 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 vs. Soft Margin SVM



- Soft-Margin also <u>always</u> has a solution
- Soft-Margin is more robust to outliers
  - Smoother surfaces (in the non-linear case)
- Hard-Margin does not require to guess the cost parameter (requires no parameters at all)

# Hard vs Soft Margin SVM



#### The old formulation:

```
Find w and b such that \mathbf{\Phi}(\mathbf{w}) = \frac{1}{2} \mathbf{w}^{\mathrm{T}} \mathbf{w} \text{ 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 \sum_{i} \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  $\alpha_i$ .
- 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  $\mathbf{Q}(\alpha) = \Sigma \alpha_i - \frac{1}{2} \Sigma \Sigma \alpha_i \alpha_j y_i y_j \mathbf{x_i}^T \mathbf{x_j}$  is maximized and (1)  $\Sigma \alpha_i y_i = \mathbf{0}$ 

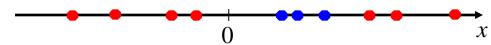
(2)  $0 \le \alpha_i \le C$  for all  $\alpha_i$ 

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

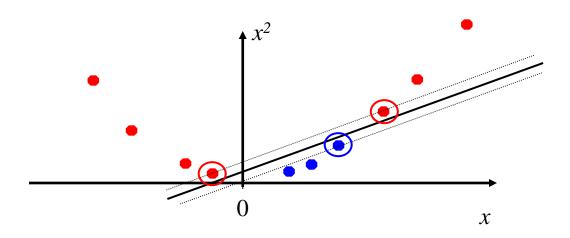
## Non-linear SVMs



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



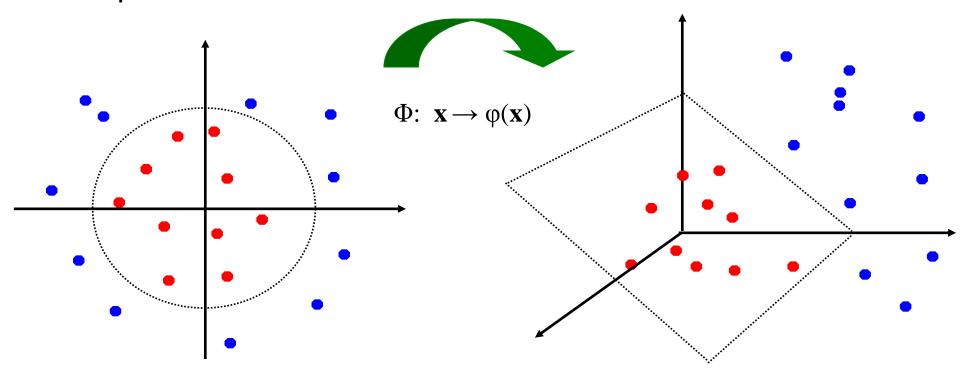
How about... mapping data to a higher-dimensional space:



# Non-linear SVMs: Feature spaces

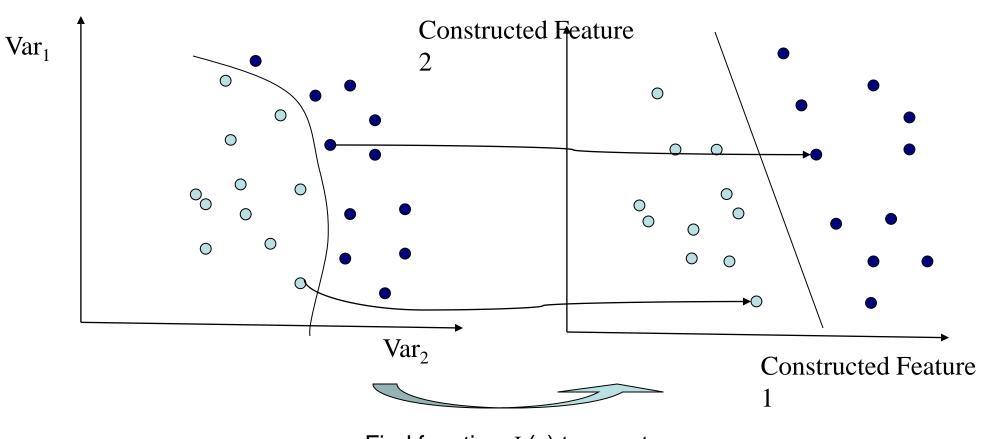


General idea: the original input space can always be mapped to some higher-dimensional feature space where the training set is separable:



# Linear Classifiers in High-Dimensional Spaces





Find function  $\Phi(x)$  to map to a different space

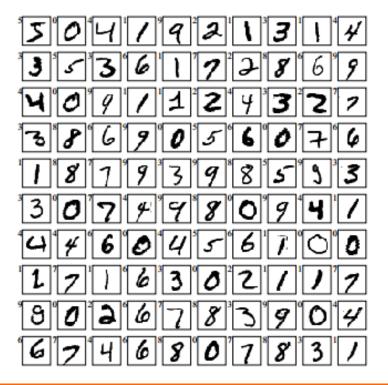
## Some problems need non-linear SVMs.



For example MNIST hand-writing recognition. 60,000 training examples, 10000 test examples, 28x28.

Linear SVM has around 8.5% test error.

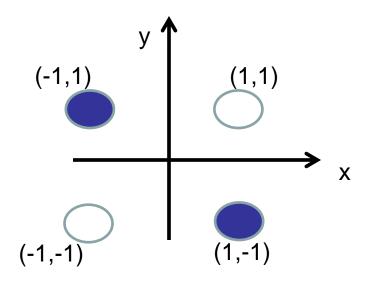
Polynomial SVM has around 1% test error.

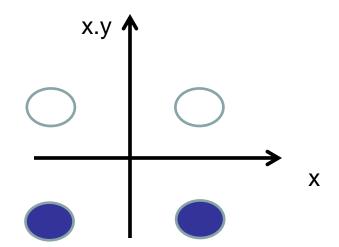




### **Linear Separation of XOR**







- XOR is not linearly separable in x,y space
- Linearly separable in x.y space
  - The kernel here will be K(x,y) = x.y

### **Nonlinear SVM - Overview**

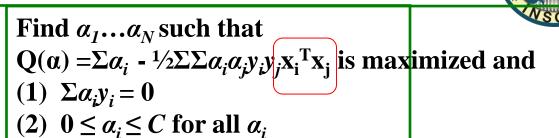


- SVM locates a separating hyperplane in the feature space and classify points in that space
- It does not need to represent the space explicitly, simply by defining a kernel function
- The kernel function plays the role of the dot product in the feature space.



### **A Little More on Kernel Functions**

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



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

- If we map the input vectors into a very high-dimensional feature space, surely the task of finding the maximummargin separator becomes computationally intractable?
  - The mathematics is all linear, which is good.
  - But the vectors have a huge number of components.
     Taking the scalar product of two vectors is very expensive.
- We can keep things tractable by using "the kernel trick"

#### The Kernel Trick

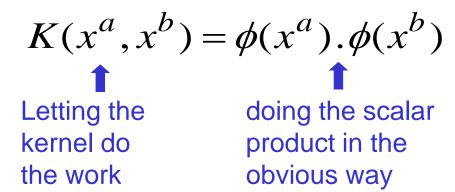
- All computations needed for the maximum-margin separator are in terms of scalar products between pairs of data points (in the highdimensional feature space).
- Scalar products are the only part of the computation that depends on the dimensionality of the high-dimensional space.
  - So if we had a fast way to do the scalar products we would not have to pay a price for solving the learning problem in the high-D space.
- The kernel trick is a way of doing scalar products a whole lot faster than is usually possible.
  - It relies on choosing a way of mapping to the high-dimensional feature space that allows fast scalar products.

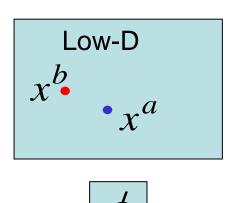


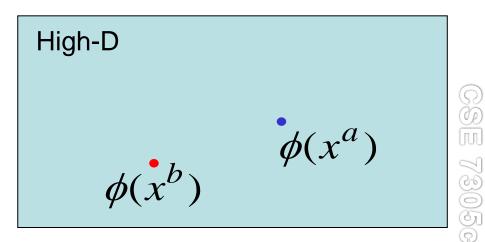
#### The kernel trick



 For many mappings from a low-D space to a high-D space, there is a simple operation on two vectors in the low-D space that can be used to compute the scalar product of their two images in the high-D space.







# Examples of Kernel Functions



- Linear:  $K(\mathbf{x_i}, \mathbf{x_j}) = \mathbf{x_i}^T \mathbf{x_j}$
- Polynomial of power p:  $K(\mathbf{x_i}, \mathbf{x_j}) = (1 + \mathbf{x_i}^T \mathbf{x_j})^p$
- Gaussian (radial-basis function network):

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

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

### Many Kernel Functions Possible



Linear Kernel

Polynomial Kernel

Gaussian Kernel

**Exponential Kernel** 

Laplacian Kernel

**ANOVA Kernel** 

Hyperbolic Tangent (Sigmoid) Kernel

Rational Quadratic Kernel

Multiquadric Kernel

Inverse Multiquadric Kernel

Circular Kernel

Spherical Kernel

Wave Kernel

**Power Kernel** 

Log Kernel

Spline Kernel

**B-Spline Kernel** 

**Bessel Kernel** 

Cauchy Kernel

Chi-Square Kernel

Histogram Intersection Kernel

Generalized Histogram Intersection Kernel

Generalized T-Student Kernel

Bayesian Kernel

Wavelet Kernel

http://crsouza.blogspot.com/2010/03/kernel-functions-for-machine-learning.html

## **Properties of SVM**



- Flexibility in choosing a similarity function
- Efficiency 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



### Multi class SVM



- We studied 2 class SVMs
- Multi class is possible using Kesler's construction
  - Input data modified as below:

$$n_{y2} = \begin{bmatrix} y \\ -y \\ 0 \\ \dots \\ 0 \end{bmatrix} n_{y3} = \begin{bmatrix} y \\ 0 \\ -y \\ \dots \\ 0 \end{bmatrix} n_{ym} = \begin{bmatrix} y \\ 0 \\ 0 \\ \dots \\ -y \end{bmatrix} \quad \text{y is a sample of class 1} \\ \text{If original problem has "m" classes, n samples, d dimensions} \\ \text{Total number of samples will become (m-1).n} \\ \text{Dimensionality will become m.d}$$

- SVM is trained on this data

Dimensionality will become m.d

http://www.insofe.edu.in

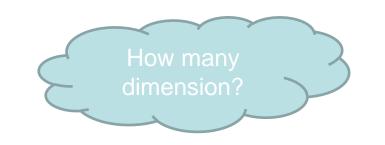
### **Multi class SVM**



- Kesler's construction not practical:
  - Sparsely populated classes
  - Similar/Confusing classes
- Train several 2 class SVMs, perform voting
- Train 1 vs all other SVMs, select best result
- Decision tree SVM !!!

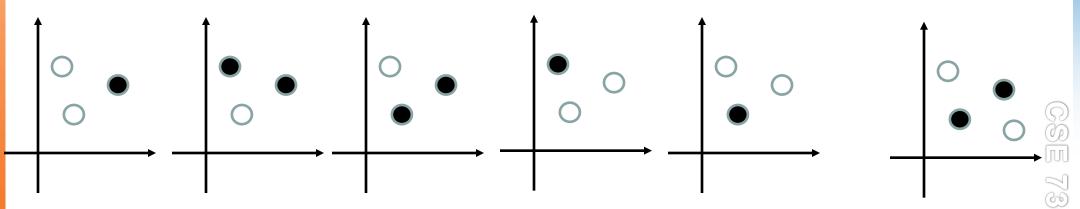


### **VC Dimension**





- Vapnic Chervonenkis Dimension
  - Explanation in plain English: Given a hyperplane in N dimensions, how many points can it separate? Ans: N+1



A line can be drawn to separate the five point sets on left, but not for points on right

http://www.autonlab.org/tutorials/vcdim08.pdf

https://alliance.seas.upenn.edu/~cis520/wiki/index.php?n=Recitations.VCDim http://www.doc.ic.ac.uk/~dfg/ProbabilisticInference/IDAPILecture18.pdf

### **VC Dimension**



 Given a classifier whose error rate on R training samples is known, and whose VC dimension is h, it is shown that error rate on an unknown test data:

$$Test\ error, e \leq Train\ error + \sqrt{\frac{h\left(\log\left(\frac{2R}{h}\right) + 1\right) - \log\left(\frac{\eta}{4}\right)}{R}}$$
 Probability of error rate being e: 1-  $\eta$ 

A linear classifier operating in h-1 dimensions has VC dimension of h

http://www.liaolin.com/Courses/vc-dimension.pdf

http://www.autonlab.org/tutorials/vcdim08.pdf

#### Resources



- 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/software

- Quadratic programming basics:
  - http://www.akiti.ca/QuadProgEx0Constr.html
  - <a href="http://www.solver.com/linear-quadratic-programming">http://www.solver.com/linear-quadratic-programming</a>
- Non-convex SVM:
  - http://web.mit.edu/seyda/www/Papers/TPAMI11\_Nonconvex.pdf





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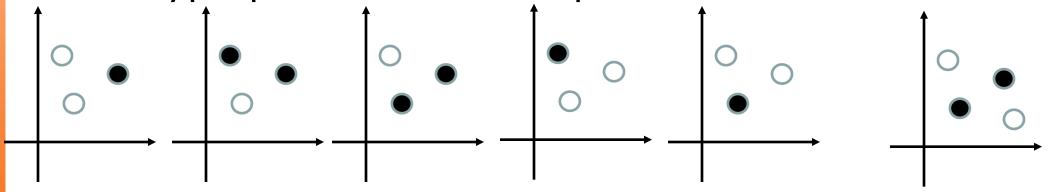
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### **VC Dimension**



- Vapnic Chervonenkis Dimension
  - Explanation in plain English: Given a data set of N points in two classes, what is the dimension which will contain at least one hyperplane that can separate the two classes?



A line can be drawn to separate the five point sets on left, but not for points on right