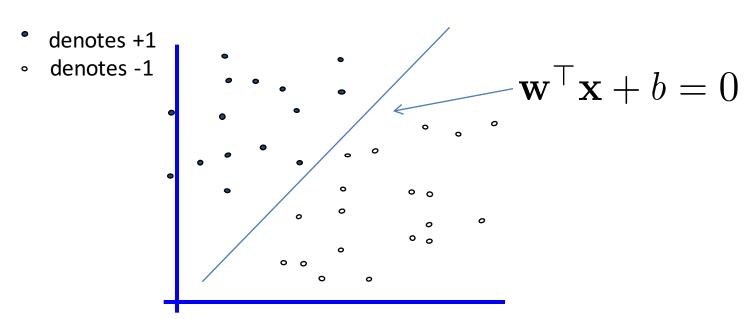
## **Support Vector Machine**

Jiayu Zhou

#### **Linear Classifiers**

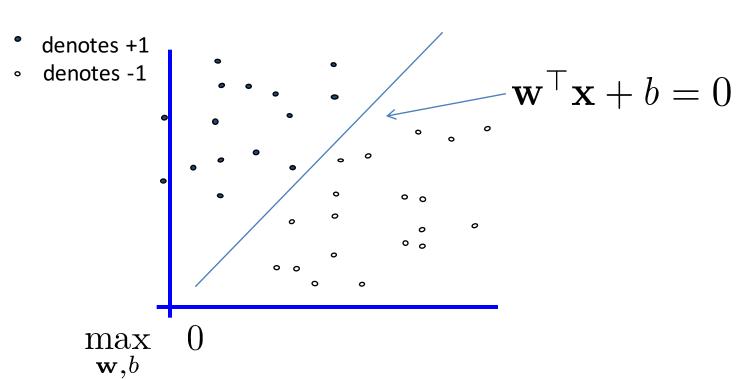
$$f(\mathbf{x}) = \operatorname{sgn}(\mathbf{w}^{\top}\mathbf{x} + b)$$



 How to find the linear decision boundary that linearly separates data points from two classes?

#### **Linear Classifiers**

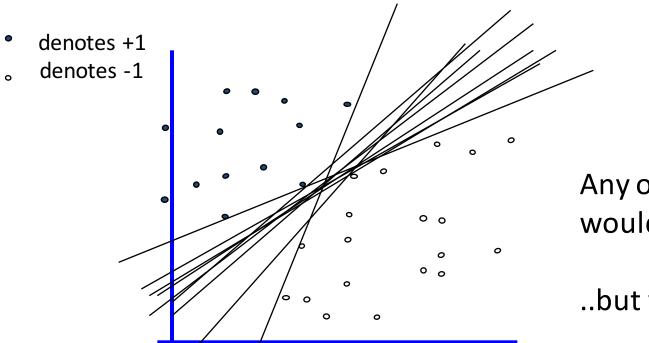
$$f(\mathbf{x}) = \operatorname{sgn}(\mathbf{w}^{\top}\mathbf{x} + b)$$



s. t. 
$$y_i(\mathbf{w}^{\top}\mathbf{x}_i + b) > 0, i = 1, ..., N$$

#### **Linear Classifiers**

$$f(\mathbf{x}) = \operatorname{sgn}(\mathbf{w}^{\top}\mathbf{x} + b)$$



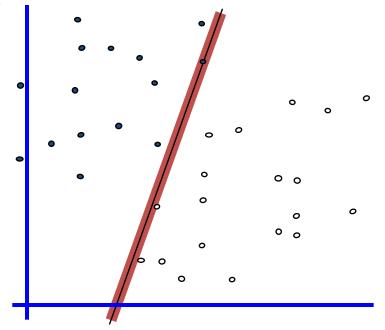
Any of these would be fine..

..but which is best?

#### Classifier Margin

$$f(\mathbf{x}) = \operatorname{sgn}(\mathbf{w}^{\top}\mathbf{x} + b)$$

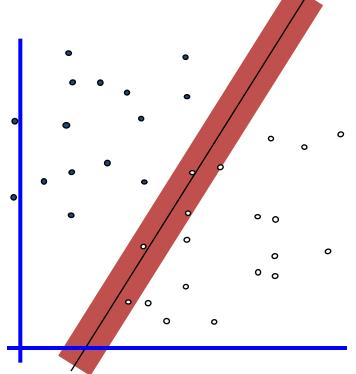
- denotes +1
- denotes -1



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

$$f(\mathbf{x}) = \operatorname{sgn}(\mathbf{w}^{\top}\mathbf{x} + b)$$

- denotes +1
- 。 denotes -1



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

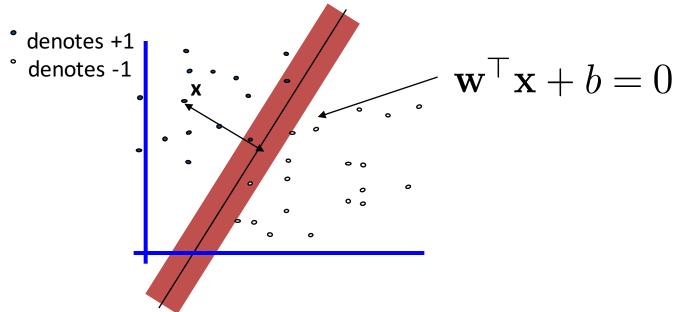
This is the simplest kind of SVM (called an Linear SVM)

## Why Maximum Margin?

$$f(\mathbf{x}) = \operatorname{sgn}(\mathbf{w}^{\top}\mathbf{x} + b)$$

- denotes +1denotes -1
- ° 0
- 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.
- 2. There's some theory (using VC dimension) that is related to (but not the same as) the proposition that this is a good thing.
- 3. Empirically it works very very well.

## Estimate the Margin

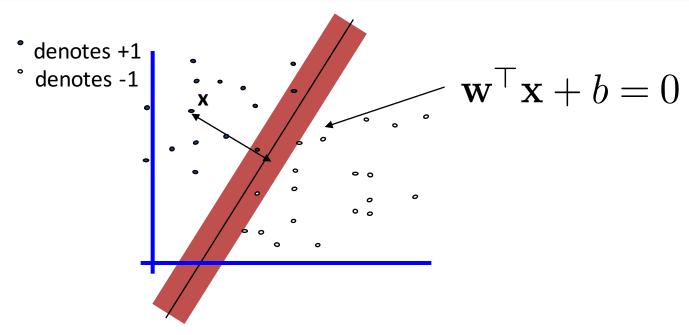


• What is the distance expression for a point x to a line

$$\mathbf{wx+b=0?}$$

$$d(\mathbf{x},\mathbf{w},b) = \frac{|\mathbf{x}^{\top}\mathbf{w}+b|}{|\mathbf{w}|_2} = \frac{|\mathbf{x}^{\top}\mathbf{w}+b|}{\sqrt{\sum_{j=1}^{d}w_j^2}}$$

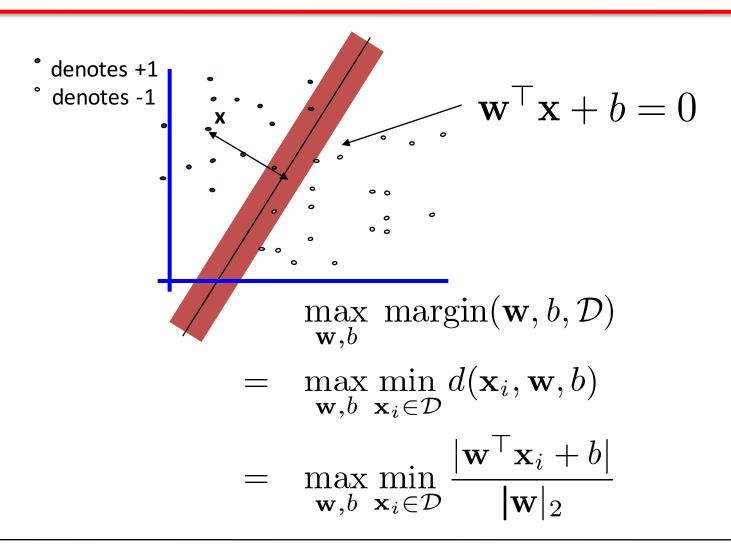
## Estimate the Margin

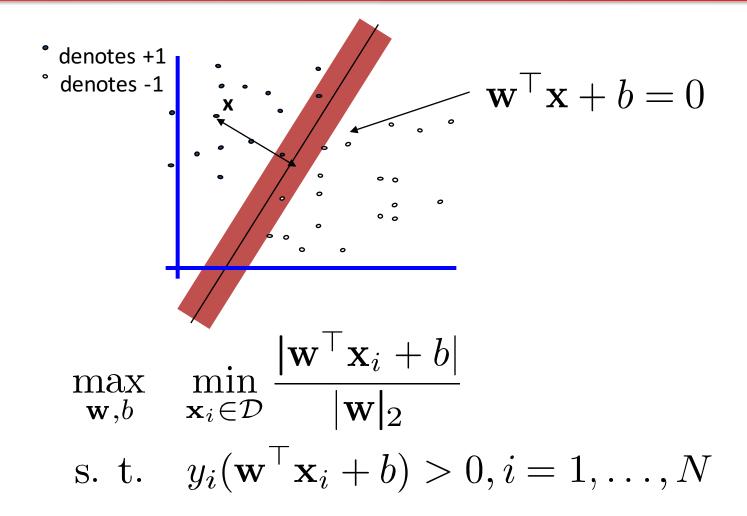


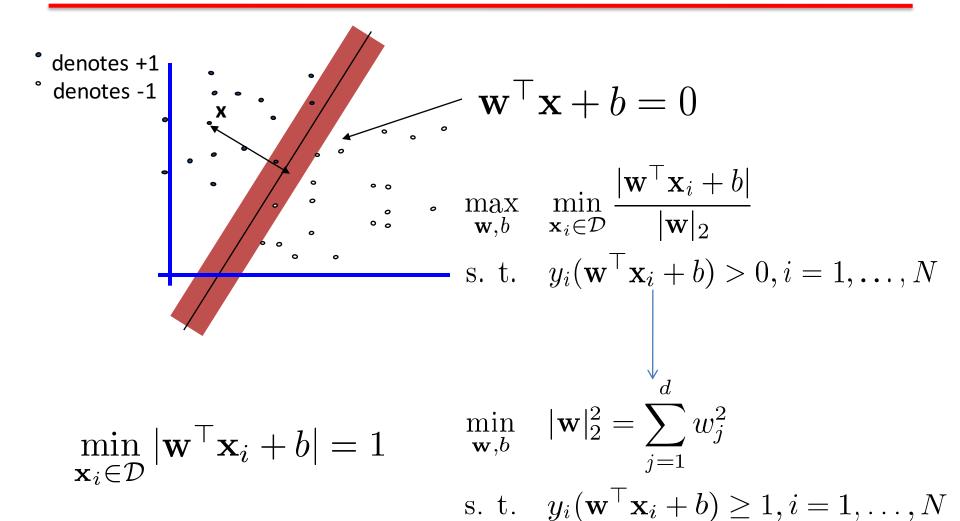
What is the classification margin for wx+b= 0?

$$\operatorname{margin}(\mathbf{w}, b, \mathcal{D}) = \min_{\mathbf{x}_i \in \mathcal{D}} d(\mathbf{x}_i, \mathbf{w}, b)$$

## Maximize the Classification Margin







$$\begin{aligned} & \min_{\mathbf{w}, b} & |\mathbf{w}|_2^2 = \sum_{j=1}^d w_j^2 \\ & \text{s. t.} & y_i(\mathbf{w}^\top \mathbf{x}_i + b) \geq 1, i = 1, \dots, N \end{aligned}$$

#### Quadratic programming problem

- Quadratic objective function
- Linear equality and inequality constraints
- Well studied problem in OR

## Quadratic Programming

Find 
$$\underset{\mathbf{u}}{\operatorname{arg\,min}} \ c + \mathbf{d}^T \mathbf{u} + \frac{\mathbf{u}^T R \mathbf{u}}{2}$$
 Quadratic criterion 
$$a_{11} u_1 + a_{12} u_2 + \ldots + a_{1m} u_m \leq b_1$$
 
$$a_{21} u_1 + a_{22} u_2 + \ldots + a_{2m} u_m \leq b_2$$
 
$$\vdots$$
 
$$a_{n1} u_1 + a_{n2} u_2 + \ldots + a_{nm} u_m \leq b_n$$
 
$$a_{n1} u_1 + a_{n2} u_2 + \ldots + a_{nm} u_m \leq b_n$$
 Quadratic criterion 
$$a_{11} u_1 + a_{12} u_2 + \ldots + a_{1m} u_m \leq b_1$$

And subject to

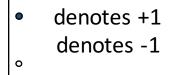
$$a_{(n+1)1}u_1 + a_{(n+1)2}u_2 + \dots + a_{(n+1)m}u_m = b_{(n+1)}$$

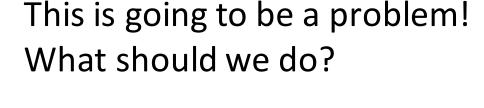
$$a_{(n+2)1}u_1 + a_{(n+2)2}u_2 + \dots + a_{(n+2)m}u_m = b_{(n+2)}$$

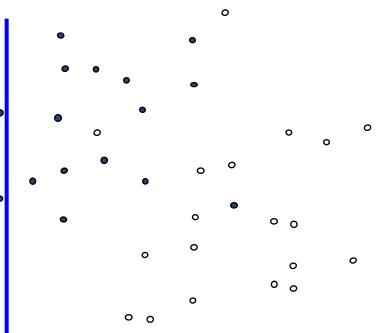
$$\vdots$$

$$a_{(n+e)1}u_1 + a_{(n+e)2}u_2 + \dots + a_{(n+e)m}u_m = b_{(n+e)}$$

 $u_{(n+e)1}u_1 + u_{(n+e)2}u_2 + \dots + u_{(n+e)m}u_m = v_{(n+e)2}u_2 + \dots + v_{(n+e)m}u_m = v_{(n+e)2}u_2 + \dots + v_{(n+e)$ 







$$\min_{\mathbf{w},b} \quad |\mathbf{w}|_2^2 = \sum_{j=1}^d w_j^2$$

s. t. 
$$y_1(\mathbf{w}^{\top}\mathbf{x}_1 + b) \ge 1$$

. . .

$$y_N(\mathbf{w}^{\top}\mathbf{x}_N + b) \ge 1$$

- denotes +1denotes -1

- Relax the constraints
- Penalize the relaxation

$$\min_{\mathbf{w},b} \quad \frac{1}{2} \sum_{j=1}^{d} w_j^2 + C \sum_{i=1}^{N} \varepsilon_i$$

s. t. 
$$y_1(\mathbf{w}^{\top}\mathbf{x}_1 + b) \ge 1 - \varepsilon_1$$

. . .

$$y_N(\mathbf{w}^{\top}\mathbf{x}_N + b) \ge 1 - \varepsilon_N$$

denotes +1denotes -1

- Relax the constraints
- Penalize the relaxation

$$\lim_{\varepsilon} \frac{1}{2} \sum_{j=1}^{d} w_j^2 + C \sum_{i=1}^{N} \varepsilon_i$$

s. t. 
$$y_1(\mathbf{w}^{\top}\mathbf{x}_1 + b) \ge 1 - \varepsilon_1, \varepsilon_1 \ge 0$$

. . .

$$y_N(\mathbf{w}^{\top}\mathbf{x}_N + b) \ge 1 - \varepsilon_N, \varepsilon_N \ge 0$$

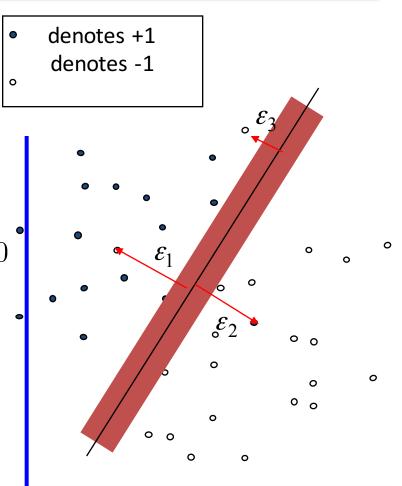
$$\min_{\mathbf{w},b,\varepsilon} \quad \frac{1}{2} \sum_{j=1}^{d} w_j^2 + C \sum_{i=1}^{N} \varepsilon_i$$

s. t. 
$$y_1(\mathbf{w}^{\top}\mathbf{x}_1 + b) \ge 1 - \varepsilon_1, \varepsilon_1 \ge 0$$

. . .

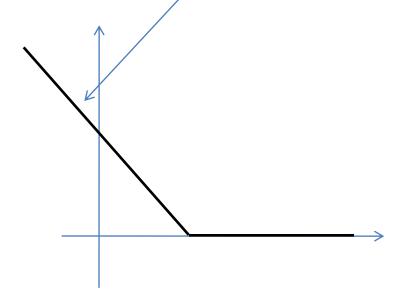
$$y_N(\mathbf{w}^{\top}\mathbf{x}_N + b) \ge 1 - \varepsilon_N, \varepsilon_N \ge 0$$

Still a quadratic programming problem



$$\min_{\mathbf{w},b} \quad \frac{1}{2} \sum_{j=1}^{d} w_j^2 + C \sum_{i=1}^{N} \ell(y_i [\mathbf{x}_i^{\top} \mathbf{w} + b])$$

Hinge loss  $\ell(z) = \max(0, 1 - z)$ 



$$\min_{\mathbf{w},b} \quad \frac{1}{2} \sum_{j=1}^{d} w_j^2 + C \sum_{i=1}^{N} \max(0, 1 - y_i [\mathbf{x}_i^{\top} \mathbf{w} + b])$$

Regularized 
$$\min_{\mathbf{w},b}$$
 regression

$$\min_{\mathbf{w},b} \frac{1}{2} \sum_{i=1}^{d} w_j^2 + C \sum_{i=1}^{N} \ln(1 + \exp(-y_i[\mathbf{x}_i^{\top} \mathbf{w} + b]))$$

#### **Dual Form of SVM**

$$\max_{\alpha_i \in [0,C]} \left\{ \sum_{i=1}^N \alpha_i - \frac{1}{2} \sum_{i,j=1}^N \alpha_i \alpha_j y_i y_j(\mathbf{x}_i^\top \mathbf{x}_j) : \sum_{i=1}^N \alpha_i y_i = 0 \right\}$$

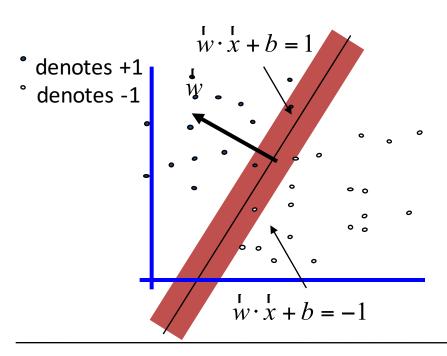
$$\mathbf{w} = \sum_{i=1}^{N} \alpha_i y_i \mathbf{x}_i$$

$$f(\mathbf{x}) = \mathbf{w}^{\mathsf{T}} \mathbf{x} + b = \sum_{i=1}^{N} \alpha_i y_i(\mathbf{x}_i^{\mathsf{T}} \mathbf{x}) + b$$

How to decide b?

#### **Dual Form of SVM**

$$\max_{\alpha_i \in [0,C]} \left\{ \sum_{i=1}^N \alpha_i - \frac{1}{2} \sum_{i,j=1}^N \alpha_i \alpha_j y_i y_j(\mathbf{x}_i^\top \mathbf{x}_j) : \sum_{i=1}^N \alpha_i y_i = 0 \right\}$$

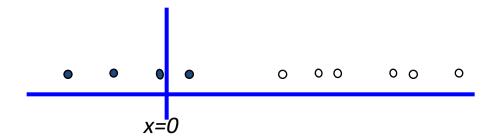


$$\alpha_i \varepsilon_i = 0, i = 1, \dots, N$$

Support vectors:  $\alpha_i > 0$ 

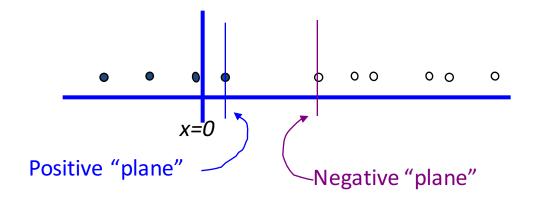
## Suppose we're in 1-dimension

What would SVMs do with this data?

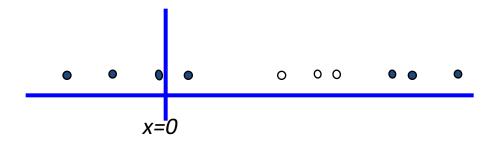


## Suppose we're in 1-dimension

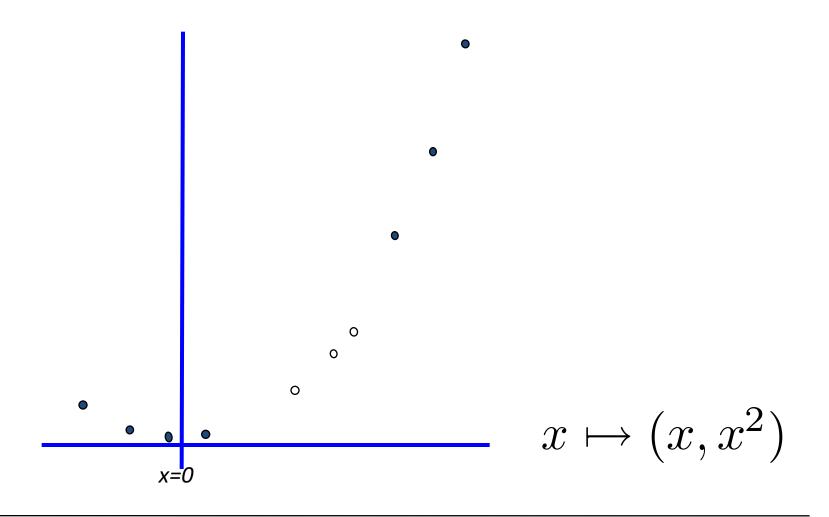
#### Not a big surprise



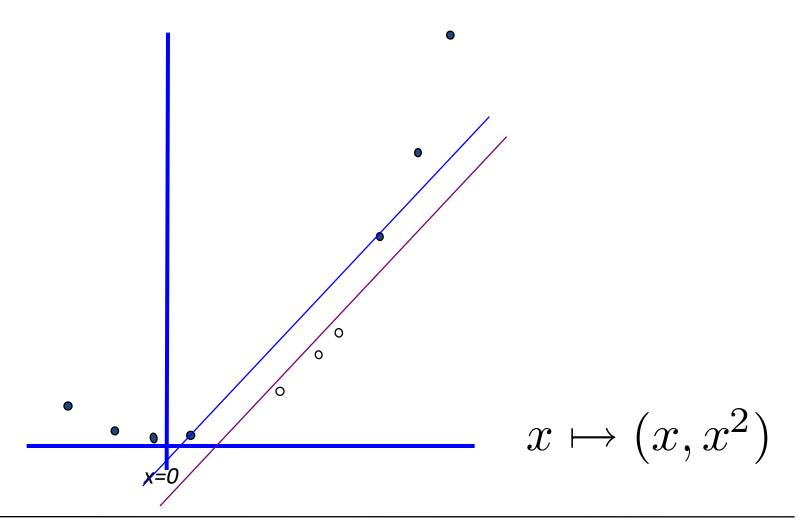
## Harder 1-dimensional Dataset



## Harder 1-dimensional Dataset



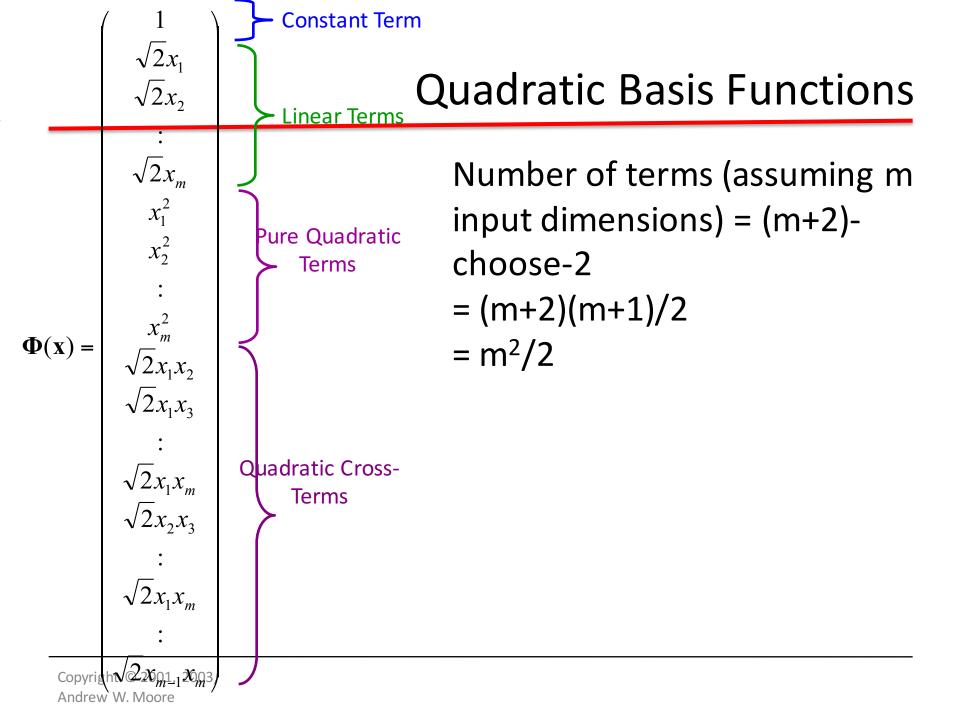
## Harder 1-dimensional Dataset



#### Common SVM Basis Functions

- Polynomial terms of x of degree 1 to q
- Radial (Gaussian) basis functions

$$\phi_j(\mathbf{x}) = \exp\left(-\frac{|\mathbf{x} - \mathbf{c}_j|_2^2}{\sigma^2}\right)$$



#### Dual Form of SVM

$$\max_{\alpha_i \in [0,C]} \left\{ \sum_{i=1}^N \alpha_i - \frac{1}{2} \sum_{i,j=1}^N \alpha_i \alpha_j y_i y_j(\mathbf{x}_i^\top \mathbf{x}_j) : \sum_{i=1}^N \alpha_i y_i = 0 \right\}$$

$$\mathbf{w} = \sum_{i=1}^{N} \alpha_i \mathbf{x}_i$$

$$f(\mathbf{x}) = \mathbf{w}^{\top} \mathbf{x} + b = \sum_{i=1}^{N} \alpha_i(\mathbf{x}_i^{\top} \mathbf{x}) + b$$

#### **Dual Form of SVM**

$$\max_{\alpha_i \in [0,C]} \left\{ \sum_{i=1}^N \alpha_i - \frac{1}{2} \sum_{i,j=1}^N \alpha_i \alpha_j y_i y_j (\vec{\phi}^\top(\mathbf{x}_i) \vec{\phi}(\mathbf{x}_j)) : \sum_{i=1}^N \alpha_i y_i = 0 \right\}$$

$$\mathbf{w} = \sum_{i=1}^{N} \alpha_i \vec{\phi}(\mathbf{x}_i)$$

$$f(\mathbf{x}) = \mathbf{w}^{\top} \mathbf{x} + b = \sum_{i=1}^{N} \alpha_i (\vec{\phi}^{\top} (\mathbf{x}_i) \vec{\phi} (\mathbf{x})) + b$$

It is computationally expensive to calculate  $\vec{\phi}^{\top}(\mathbf{x}_i)\vec{\phi}(\mathbf{x}_j)$ 

# Quadratic Dot Products

$$\Phi(a) \bullet \Phi(b) =$$

$$\begin{pmatrix} 1 \\ \sqrt{2}a_1 \\ \sqrt{2}a_2 \\ \vdots \\ \sqrt{2}a_m \\ a_1^2 \\ a_2^2 \\ \vdots \\ a_m^2 \\ \sqrt{2}a_1a_2 \\ \sqrt{2}a_1a_3 \\ \vdots \\ \sqrt{2}a_1a_m \\ \sqrt{2}a_2a_3 \\ \vdots \\ \sqrt{2}a_1a_m \\ \vdots \\ \sqrt{2}a_{m-1}a_m \end{pmatrix}$$

 $\sqrt{2}b_1 \\ \sqrt{2}b_2$  $\sqrt{2}b_{m}$  $b_1^2 \\ b_2^2$  $b_m^2$  $\sqrt{2}b_1b_2$  $\sqrt{2}b_1b_3$  $\frac{\sqrt{2}b_{\scriptscriptstyle 1}b_{\scriptscriptstyle m}}{\sqrt{2}b_{\scriptscriptstyle 2}b_{\scriptscriptstyle 3}}$  $\sqrt{2}b_{\scriptscriptstyle 1}b_{\scriptscriptstyle m}$ 

$$\begin{array}{c}
1 \\
+ \\
\sum_{i=1}^{m} 2a_{i}b_{i} \\
+ \\
\sum_{i=1}^{m} a_{i}^{2}b_{i}^{2} \\
+ \\
\sum_{i=1}^{m} \sum_{j=i+1}^{m} 2a_{i}a_{j}b_{i}b_{j}
\end{array}$$

## Quadratic Dot Products

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

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

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

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

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

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

$$= \sum_{i=1}^{m} (a_{i}b_{i})^{2} + 2\sum_{i=1}^{m} \sum_{j=i+1}^{m} a_{i}b_{i}a_{j}b_{j} + 2\sum_{i=1}^{m} a_{i}b_{i} + 1$$

#### **Kernel Trick**

$$\max_{\alpha_i \in [0,C]} \left\{ \sum_{i=1}^N \alpha_i - \frac{1}{2} \sum_{i,j=1}^N \alpha_i \alpha_j y_i y_j (\vec{\phi}^\top(\mathbf{x}_i) \vec{\phi}(\mathbf{x}_j)) : \sum_{i=1}^N \alpha_i y_i = 0 \right\}$$

$$\mathbf{w} = \sum_{i=1}^{N} \alpha_i \vec{\phi}(\mathbf{x}_i)$$

$$f(\mathbf{x}) = \mathbf{w}^{\top} \mathbf{x} + b = \sum_{i=1}^{N} \alpha_i (\vec{\phi}^{\top} (\mathbf{x}_i) \vec{\phi} (\mathbf{x})) + b$$

Define a kernel function:  $\kappa(\mathbf{x}_i, \mathbf{x}_j) = \vec{\phi}^{\top}(\mathbf{x}_i) \vec{\phi}(\mathbf{x}_j)$ 

#### **Kernel Trick**

$$\max_{\alpha_i \in [0,C]} \left\{ \sum_{i=1}^N \alpha_i - \frac{1}{2} \sum_{i,j=1}^N \alpha_i \alpha_j y_i y_j \kappa(\mathbf{x}_i, \mathbf{x}_j) : \sum_{i=1}^N \alpha_i y_i = 0 \right\}$$

$$\mathbf{w} = \sum_{i=1}^{N} \alpha_i \vec{\phi}(\mathbf{x}_i)$$

$$f(\mathbf{x}) = \mathbf{w}^{\top} \mathbf{x} + b = \sum_{i=1}^{N} \alpha_i \kappa(\mathbf{x}_i, \mathbf{x}) + b$$

Define a kernel function:  $\kappa(\mathbf{x}_i, \mathbf{x}_j) = \vec{\phi}^{\top}(\mathbf{x}_i) \vec{\phi}(\mathbf{x}_j)$ 

#### **SVM Kernel Functions**

Polynomial kernel function

$$\kappa(\mathbf{x}_i, \mathbf{x}_j) = (\mathbf{x}_i^\top \mathbf{x}_j + 1)^q$$

Radial basis kernel function (universal kernel)

$$\kappa(\mathbf{x}_i, \mathbf{x}_j) = \exp\left(-\lambda |\mathbf{x}_i - \mathbf{x}_j|_2^2\right)$$

#### **Kernel Tricks**

Replacing dot product with a kernel function

$$\kappa(\mathbf{x}_i, \mathbf{x}_j) = \vec{\phi}^{\top}(\mathbf{x}_i) \vec{\phi}(\mathbf{x}_j)$$

- Not all functions are kernel functions
- Are they kernel functions?

$$\kappa(\vec{a}, \vec{b}) = \sum_{i=1}^{d} (a_i - b_i)^3$$

$$\kappa(\vec{a}, \vec{b}) = \sum_{i=1}^{d} (a_i - b_i)^4 (a_i + b_i)^2$$

### **Kernel Tricks**

#### Mercer's condition

To expand Kernel function k(x,y) into a dot product, i.e.  $k(x,y)=\Phi(x)\cdot\Phi(y)$ , k(x,y) has to be positive semi-definite function, i.e., for any function f(x) whose  $\int f^2(x)dx$  is finite, the following inequality holds

$$\int d\mathbf{x}_a d\mathbf{x}_b f(\mathbf{x}_a) \kappa(\mathbf{x}_a, \mathbf{x}_b) f(\mathbf{x}_b) \ge 0$$

### **Kernel Tricks**

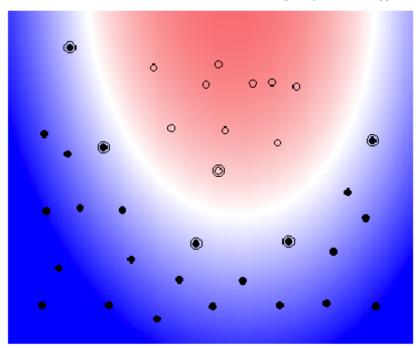
- Introducing nonlinearity into the model
- Computationally efficient

## Nonlinear Kernel (I)

#### **Example: SVM with Polynomial of Degree 2**

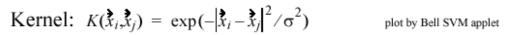
Kernel:  $K(x_i, x_j) = [x_i \cdot x_j + 1]^2$ 

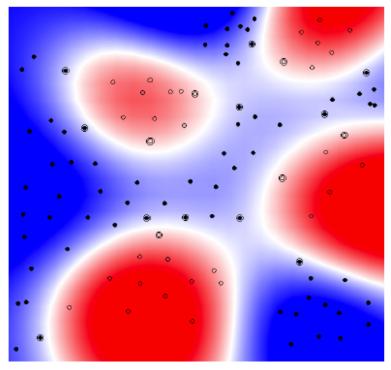
plot by Bell SVM applet



# Nonlinear Kernel (II)

#### **Example: SVM with RBF-Kernel**





## Reproducing Kernel Hilbert Space (RKHS)

- Reproducing Kernel Hilbert Space H
  - Eigen decomposition:

$$\kappa(\mathbf{x}_a, \mathbf{x}_b) = \sum_{i=1}^{\infty} \gamma_i \phi_i(\mathbf{x}_a) \phi_i(\mathbf{x}_b) \qquad \gamma_i \ge 0, \sum_{i=1}^{\infty} \gamma_i^2 < \infty$$

• Elements of space *H*:

$$f(\mathbf{x}) = \sum_{i=1}^{\infty} c_i \phi_i(\mathbf{x})$$
  $\langle f, f \rangle_{\mathcal{H}} = \sum_{i=1}^{\infty} c_i^2 / \gamma_i < \infty$ 

Reproducing property

$$\langle \kappa(\mathbf{x}, \cdot), f(\cdot) \rangle_{\mathcal{H}} = f(\mathbf{x})$$

## Reproducing Kernel Hilbert Space (RKHS)

$$\min_{\mathbf{w},b} \frac{1}{2} \sum_{j=1}^{d} w_j^2 + C \sum_{i=1}^{N} \max(0, 1 - y_i [\mathbf{x}_i^{\top} \mathbf{w} + b])$$

$$\min_{f \in \mathcal{H}} \frac{1}{2} \langle f, f \rangle_{\mathcal{H}} + C \sum_{i=1}^{N} \max(0, 1 - y_i f(\mathbf{x}_i))$$

Representer theorem

## Kernelize Logistic Regression

 How can we introduce nonlinearity into the logistic regression model?

$$p(y|\mathbf{x}) = \frac{1}{1 + \exp(-y\mathbf{x}^{\top}\mathbf{w})}$$

#### **Diffusion Kernel**

- Kernel function describes the correlation or similarity between two data points
- Given that a similarity function s(x,y)
  - Non-negative and symmetric
  - Does not obey Mercer's condition
- How can we generate a kernel function based on this similarity function?

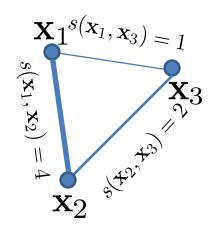
A graph theory approach ...

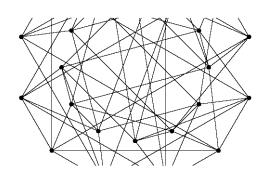
### **Diffusion Kernel**

- Create a graph for all the training examples
  - Each vertex corresponds to a data point
  - The weight of each edge is the similarity s(x,y)
- Graph Laplacian

$$L_{i,j} = \begin{cases} s(\mathbf{x}_i, \mathbf{x}_j) & i \neq j \\ -\sum_{k \neq i} s(\mathbf{x}_i, \mathbf{x}_k) & i = j \end{cases}$$

Negative semi-definite





### **Diffusion Kernel**

#### Consider a simple Laplacian

$$L_{i,j} = \begin{cases} 1 & i \neq j \\ -\sum_{k \in \mathcal{N}_i} 1 & i = j \end{cases}$$

Consider  $L^2$ ,  $L^3$ , ...

What do these matrices represent?

A diffusion kernel 
$$K_{\beta} = e^{\beta L} = \lim_{n \to \infty} \left(I + \frac{\beta}{n}L\right)^n$$

## Diffusion Kernel: Properties

$$K_{\beta} = \exp(\beta L)$$

- Positive definite
- How to compute the diffusion kernel?

## Doing Multi-class Classification

- SVMs can only handle two-class outputs (i.e. a categorical output variable with arity 2).
- What can be done?
- Answer: with output arity N, learn N SVM's

```
SVM 1 learns "Output==1" vs "Output != 1"
SVM 2 learns "Output==2" vs "Output != 2"
:
SVM N learns "Output==N" vs "Output != N"
```

 Then to predict the output for a new input, just predict with each SVM and find out which one puts the prediction the furthest into the positive region.

## Kernel Learning

$$\max_{\alpha_i \in [0,C]} \left\{ \sum_{i=1}^N \alpha_i - \frac{1}{2} \sum_{i,j=1}^N \alpha_i \alpha_j y_i y_j \kappa(\mathbf{x}_i, \mathbf{x}_j) : \sum_{i=1}^N \alpha_i y_i = 0 \right\}$$

$$f(\mathbf{x}) = \mathbf{w}^{\top} \mathbf{x} + b = \sum_{i=1}^{N} \alpha_i \kappa(\mathbf{x}_i, \mathbf{x}) + b$$

What if we have multiple kernel functions  $\kappa_1(\mathbf{x}, \mathbf{x}), \kappa_2(\mathbf{x}, \mathbf{x}), \dots, \kappa_m(\mathbf{x}, \mathbf{x})$ 

- Which one is the best?
- How can we combine multiple kernels?

## Kernel Learning

$$\kappa(\mathbf{x}, \mathbf{x}; \gamma) = \sum_{k=1}^{m} \gamma_k \kappa_k(\mathbf{x}, \mathbf{x})$$

$$\gamma = (\gamma_1, \dots, \gamma_m) \in \Delta = \left\{ \gamma \in \mathbb{R}_+^m : \sum_{k=1}^m \gamma_k = 1 \right\}$$

$$\min_{\gamma \in \Delta} \max_{\alpha_i \in [0,C]} \left\{ \sum_{i=1}^N \alpha_i - \frac{1}{2} \sum_{i,j=1}^N \alpha_i \alpha_j y_i y_j \kappa(\mathbf{x}_i, \mathbf{x}_j; \gamma) : \sum_{i=1}^N \alpha_i y_i = 0 \right\}$$

$$f(\mathbf{x}) = \mathbf{w}^{\top} \mathbf{x} + b = \sum_{i=1}^{N} \alpha_i \kappa(\mathbf{x}_i, \mathbf{x}; \gamma) + b$$

#### References

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