

# Support Vector Machines & Kernels

## BCSE3066

Instructor: Pratyush Kumar Deka

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# Outline

- Prediction
  - Why might predictions be wrong?
- Support vector machines
  - Doing really well with linear models
- Kernels
  - Making the non-linear linear

# Why Might Predictions be Wrong?

- True non-determinism
  - Flip a biased coin
  - $p(\text{heads}) = \theta$
  - Estimate  $\theta$
  - If  $\theta > 0.5$  predict ‘heads’, else ‘tails’

Lots of ML research on problems like this:

- Learn a model
- Do the best you can in expectation

# Why Might Predictions be Wrong?

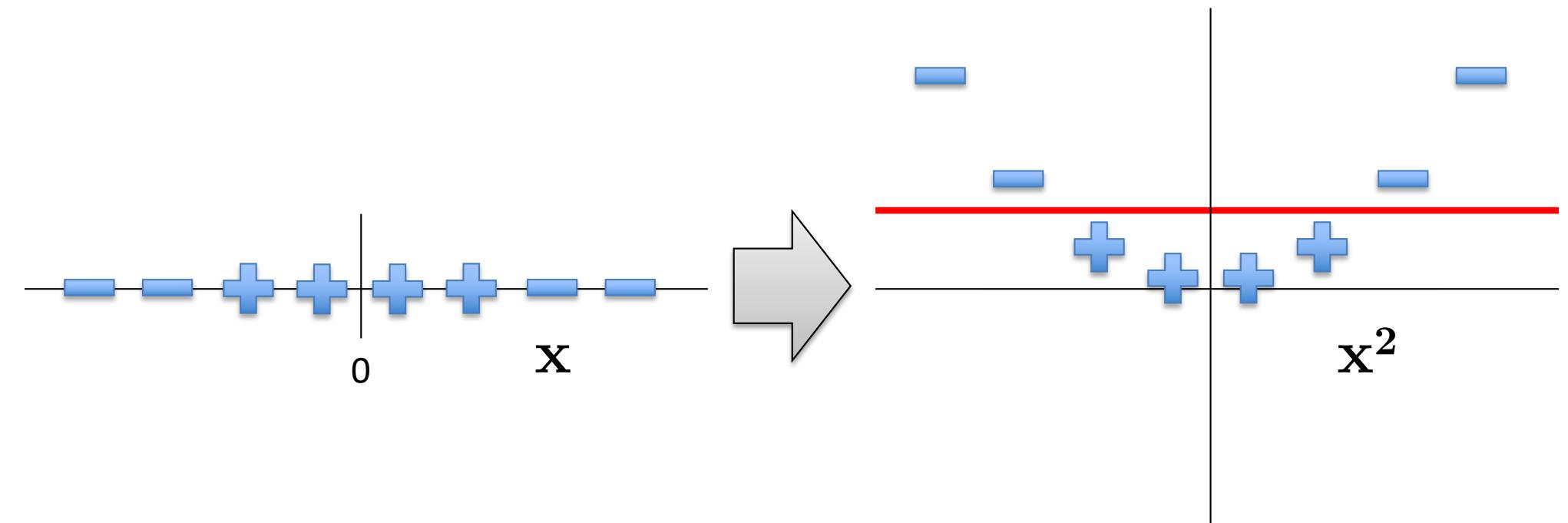
- Partial observability
  - Something needed to predict  $y$  is missing from observation  $x$
  - $N$ -bit parity problem
    - $x$  contains  $N-1$  bits (hard PO)
    - $x$  contains  $N$  bits but learner ignores some of them (soft PO)
- Noise in the observation  $x$ 
  - Measurement error
  - Instrument limitations

# Why Might Predictions be Wrong?

- True non-determinism
- Partial observability
  - hard, soft
- Representational bias
- Algorithmic bias
- Bounded resources

# Representational Bias

- Having the right features ( $x$ ) is crucial



# Support Vector Machines

Doing *Really* Well with Linear  
Decision Surfaces

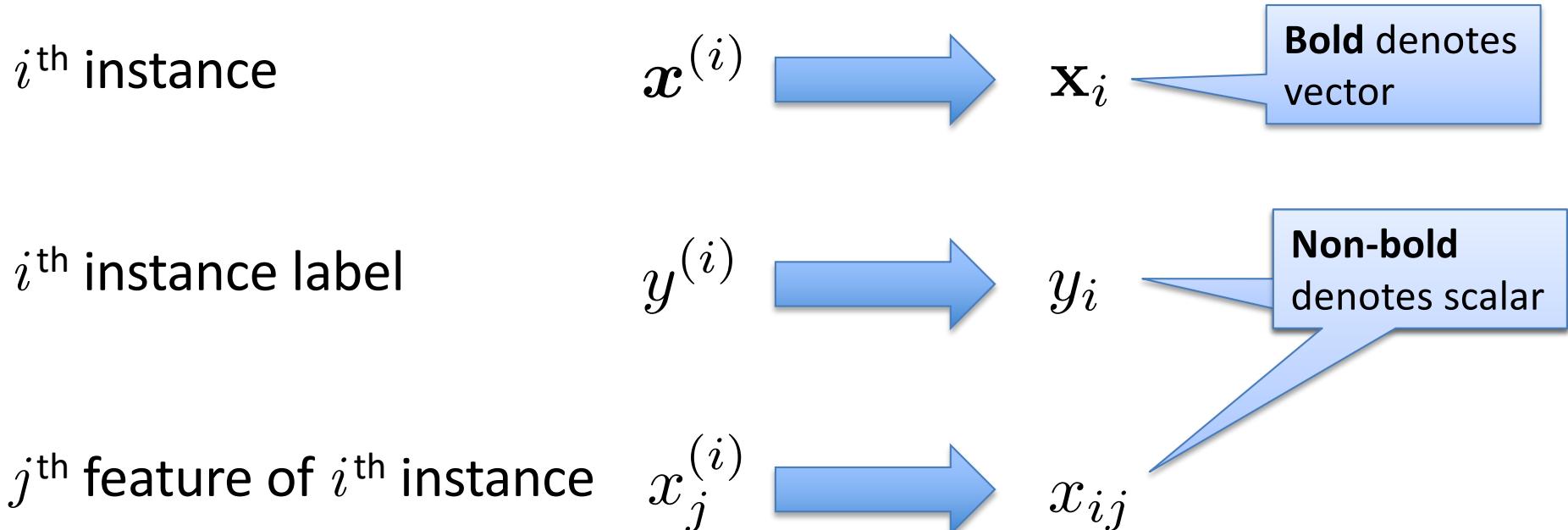
# Strengths of SVMs

- Good generalization
  - in theory
  - in practice
- Works well with few training instances
- Find globally best model
- Efficient algorithms
- Amenable to the kernel trick

# Minor Notation Change

To better match notation used in SVMs  
...and to make matrix formulas simpler

We will drop using superscripts for the  $i^{\text{th}}$  instance



# Linear Separators

- Training instances

$$\mathbf{x} \in \mathbb{R}^{d+1}, x_0 = 1$$

$$y \in \{-1, 1\}$$

- Model parameters

$$\boldsymbol{\theta} \in \mathbb{R}^{d+1}$$

- Hyperplane

$$\boldsymbol{\theta}^\top \mathbf{x} = \langle \boldsymbol{\theta}, \mathbf{x} \rangle = 0$$

- Decision function

$$h(\mathbf{x}) = \text{sign}(\boldsymbol{\theta}^\top \mathbf{x}) = \text{sign}(\langle \boldsymbol{\theta}, \mathbf{x} \rangle)$$

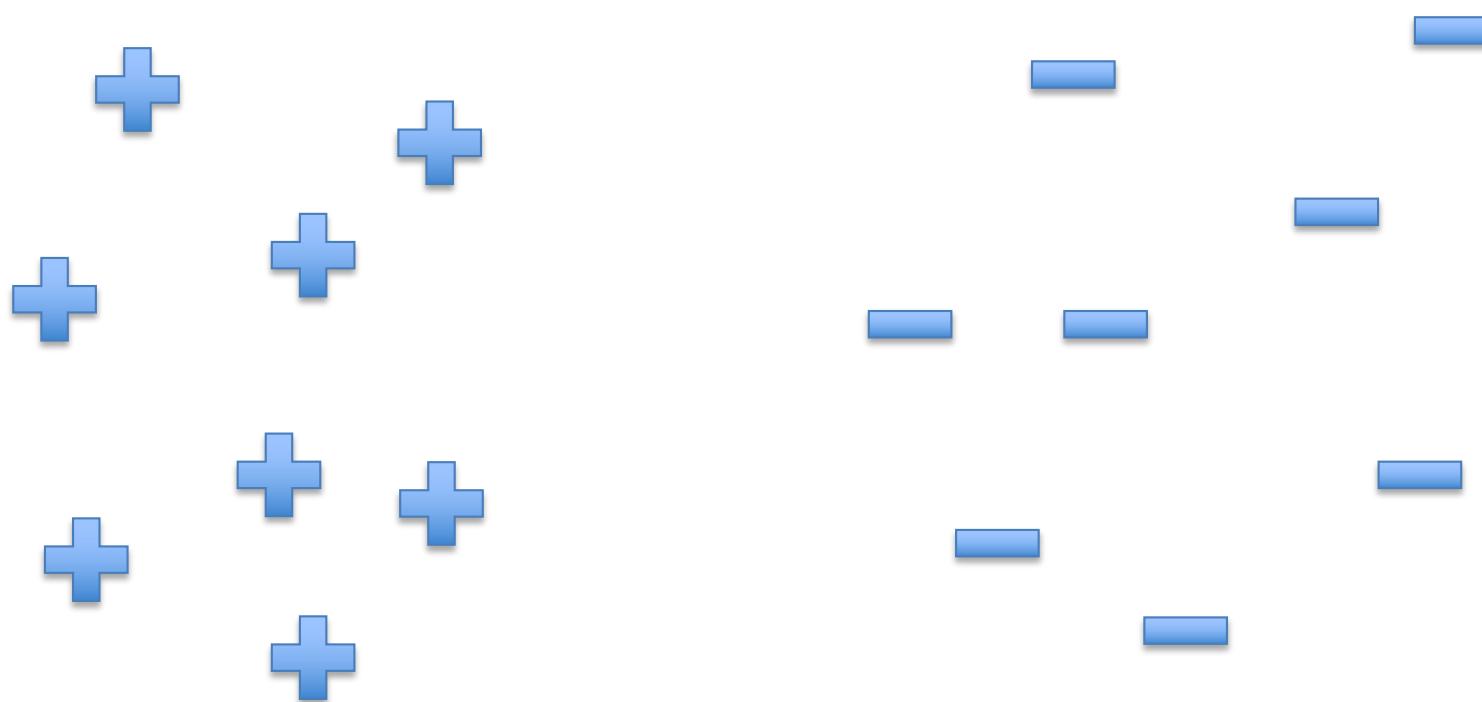
Recall:

Inner (dot) product:

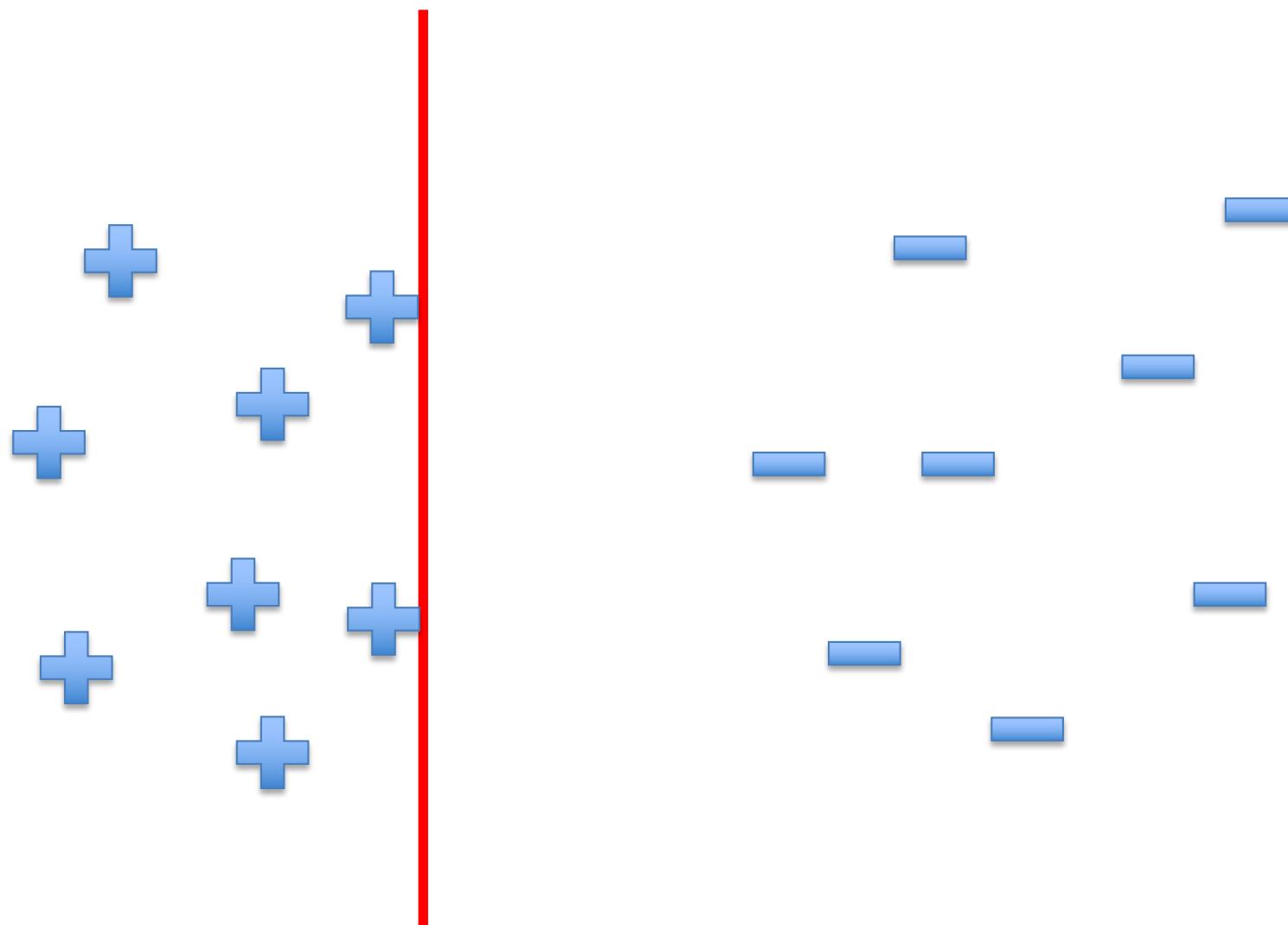
$$\langle \mathbf{u}, \mathbf{v} \rangle = \mathbf{u} \cdot \mathbf{v} = \mathbf{u}^\top \mathbf{v}$$

$$= \sum_i u_i v_i$$

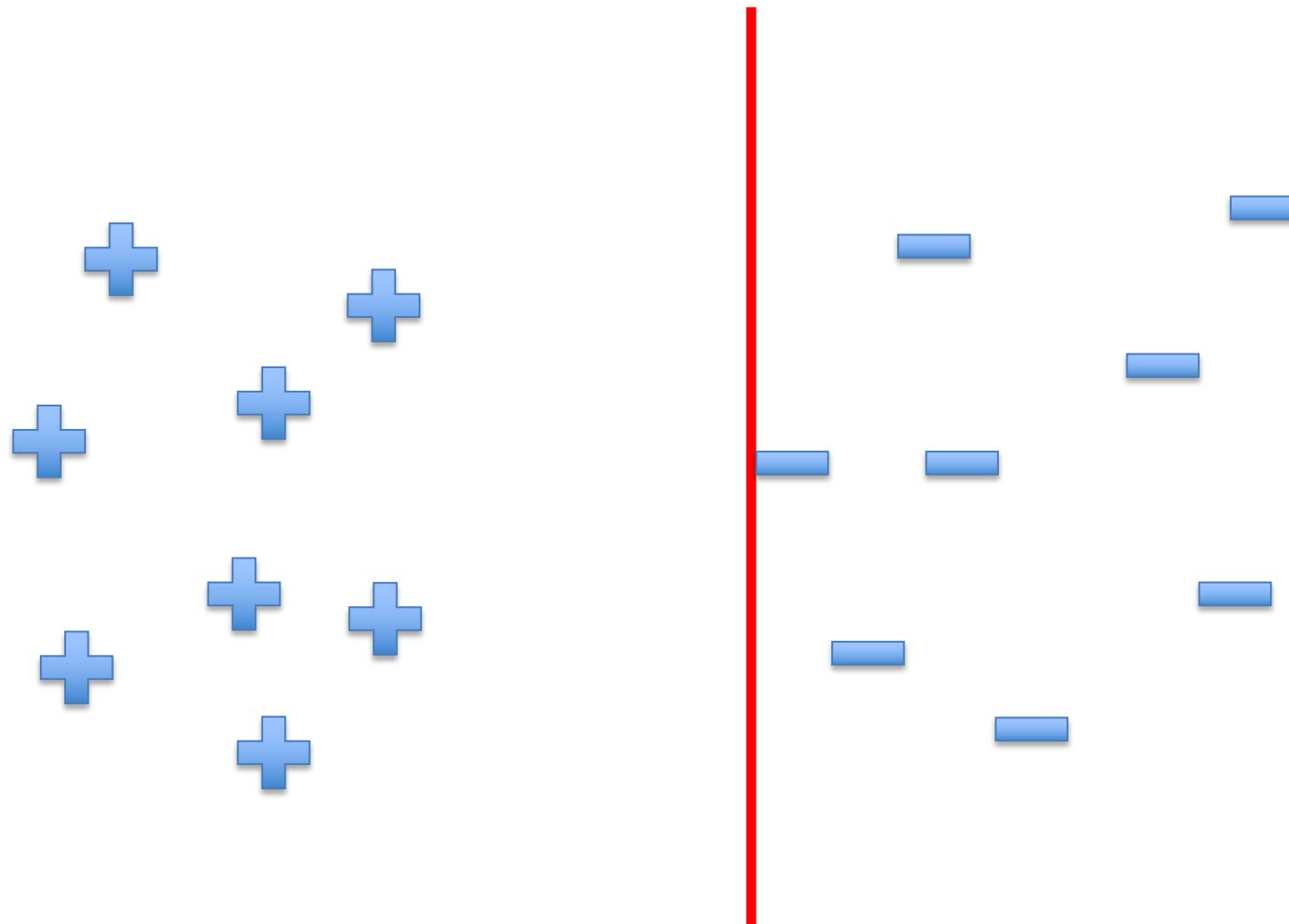
# Intuitions



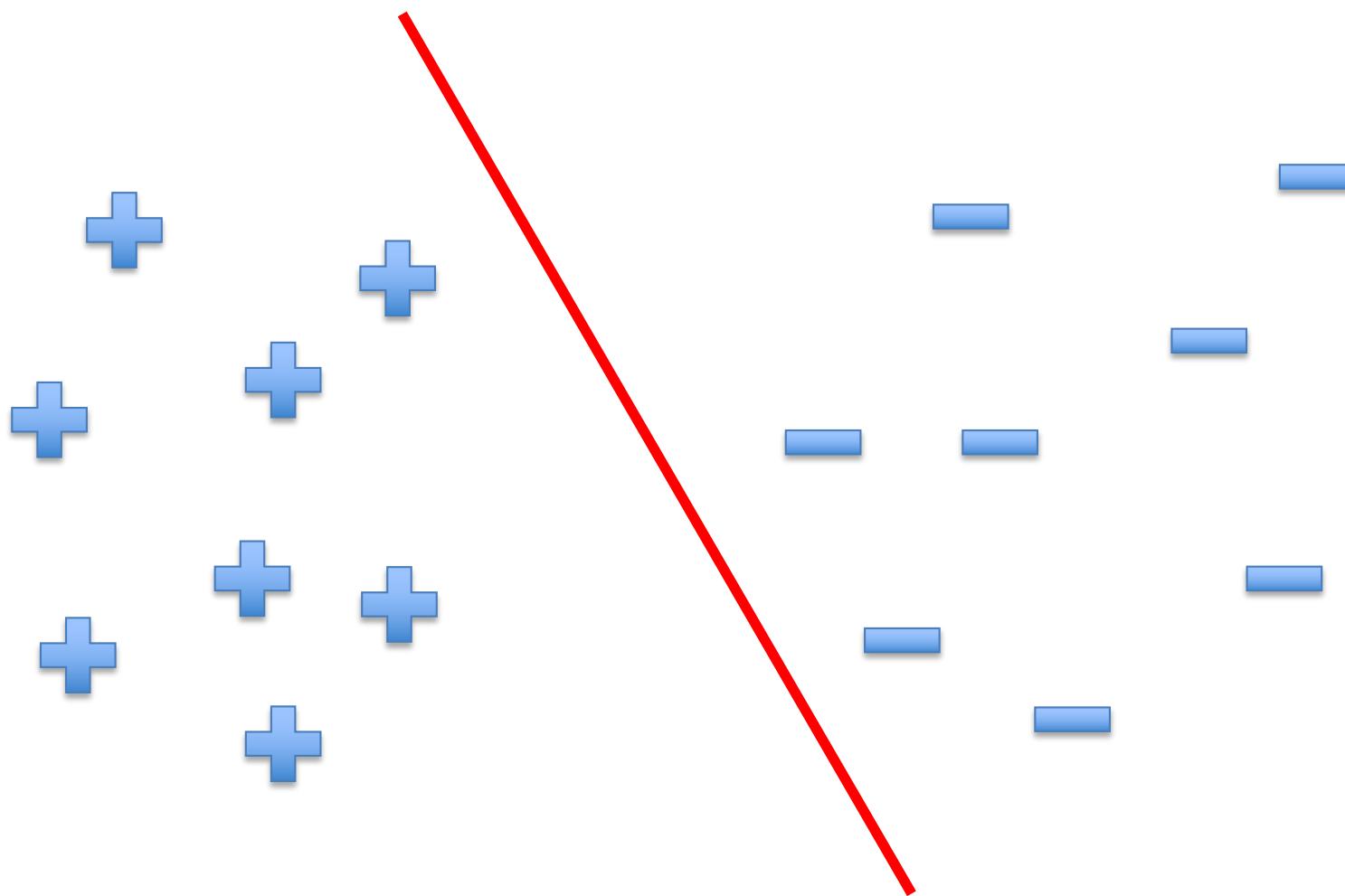
# Intuitions



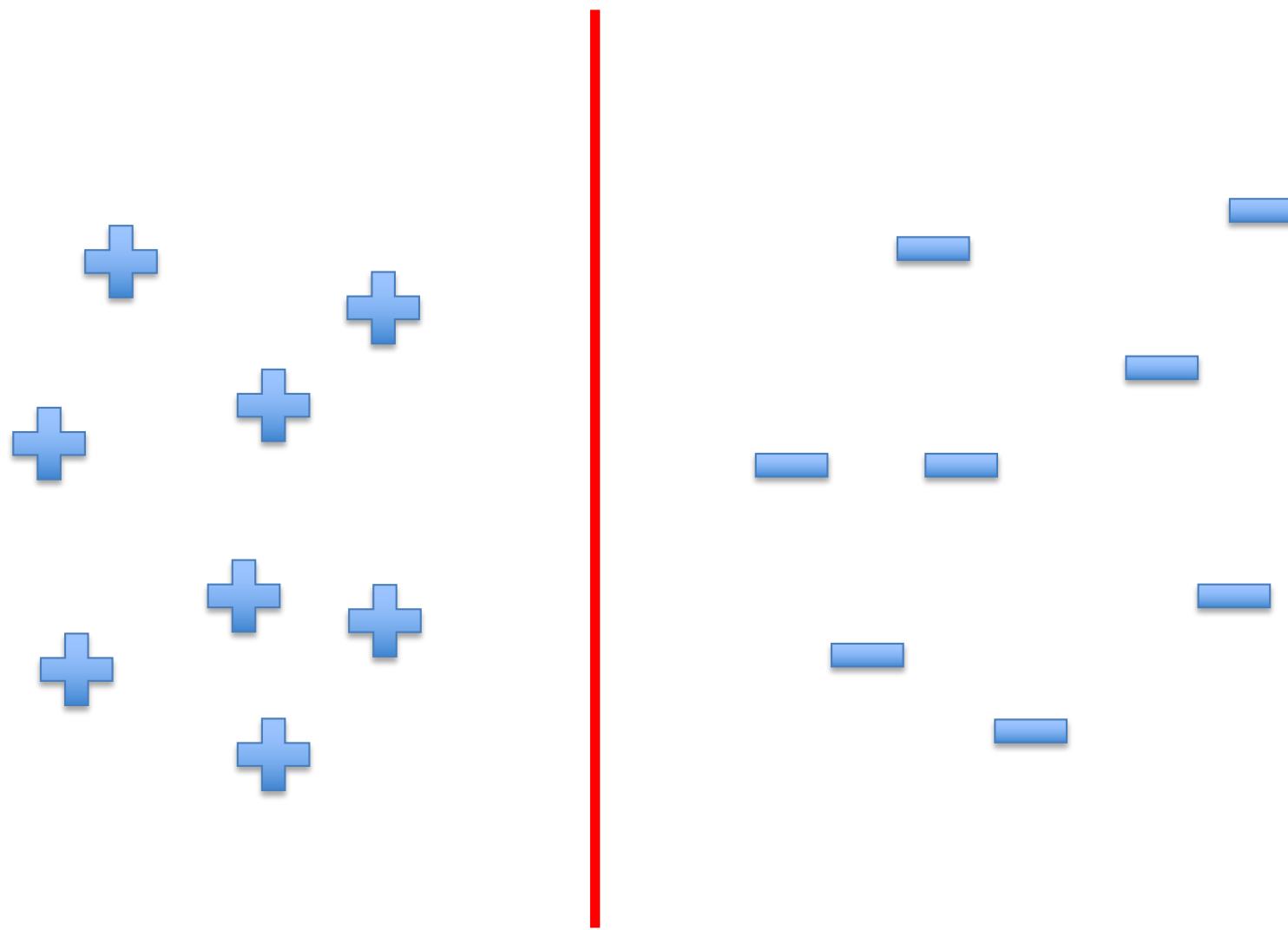
# Intuitions



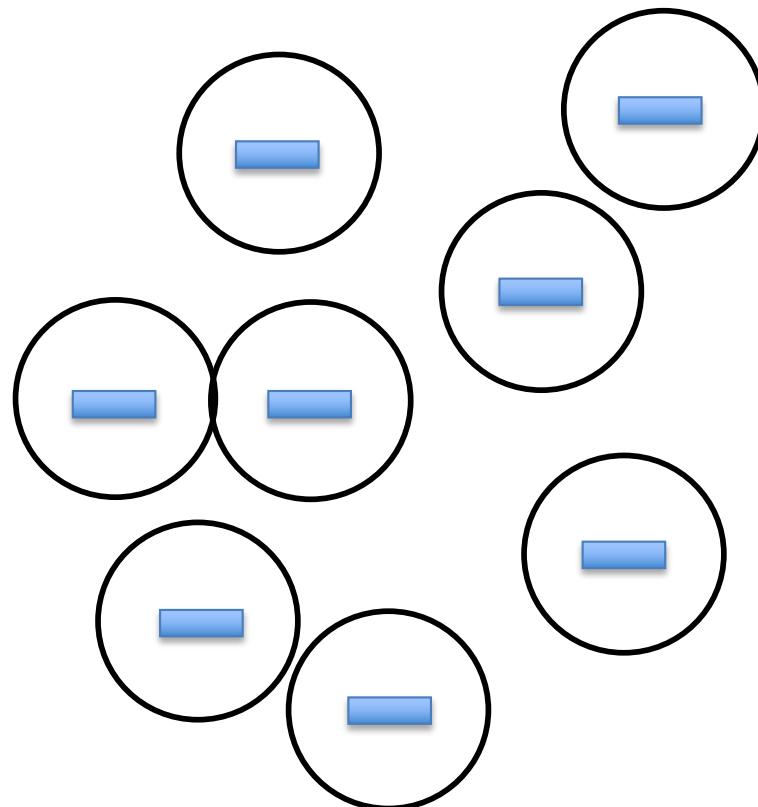
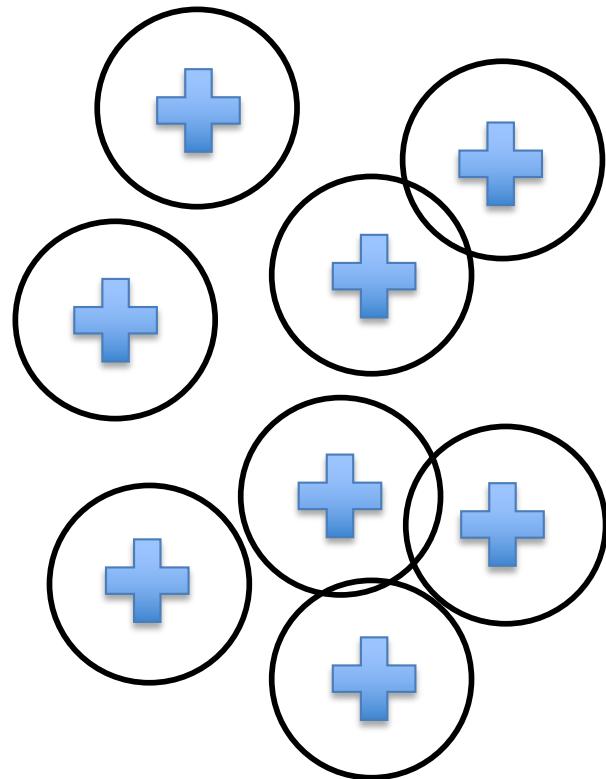
# Intuitions



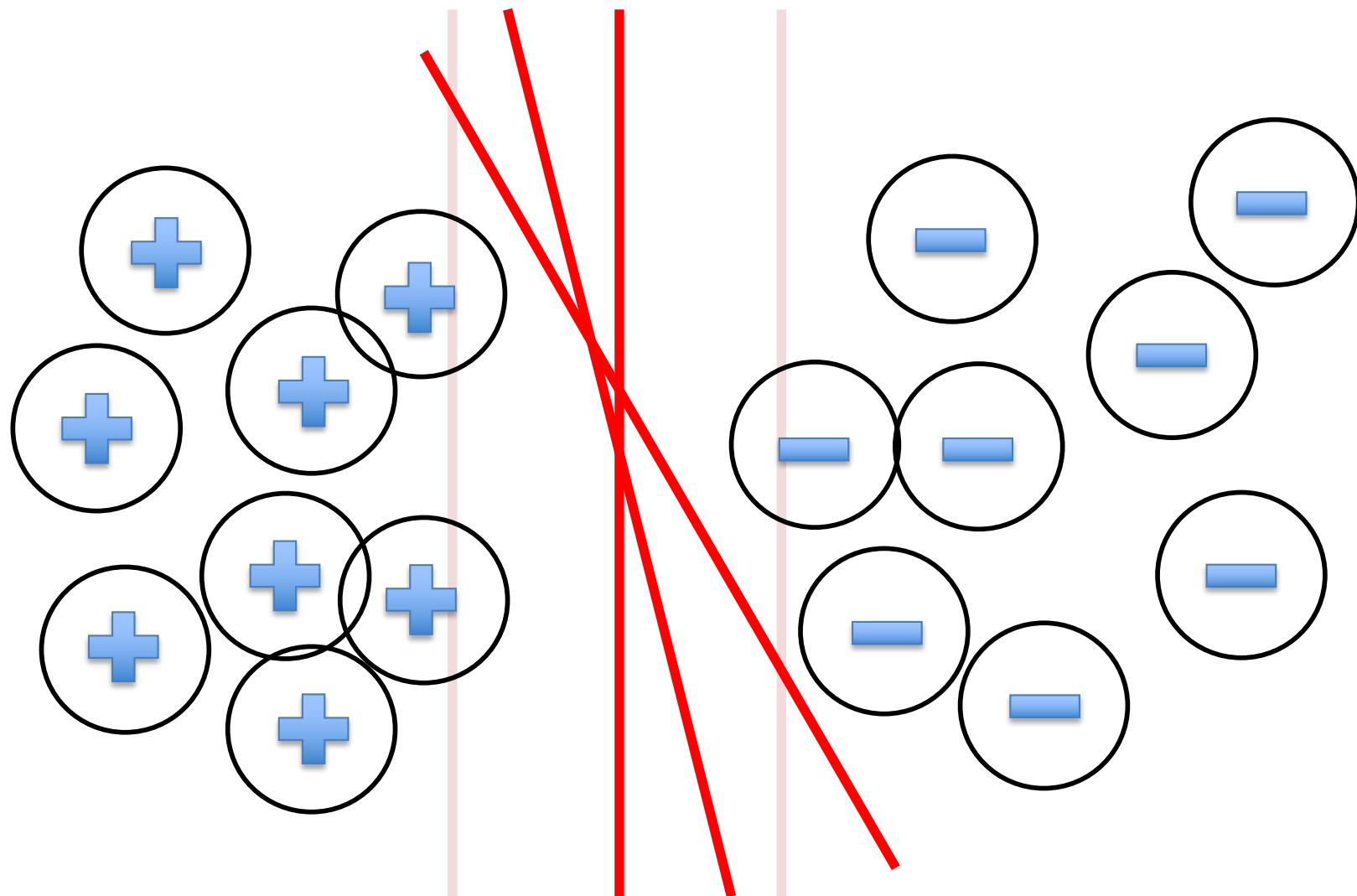
# A “Good” Separator



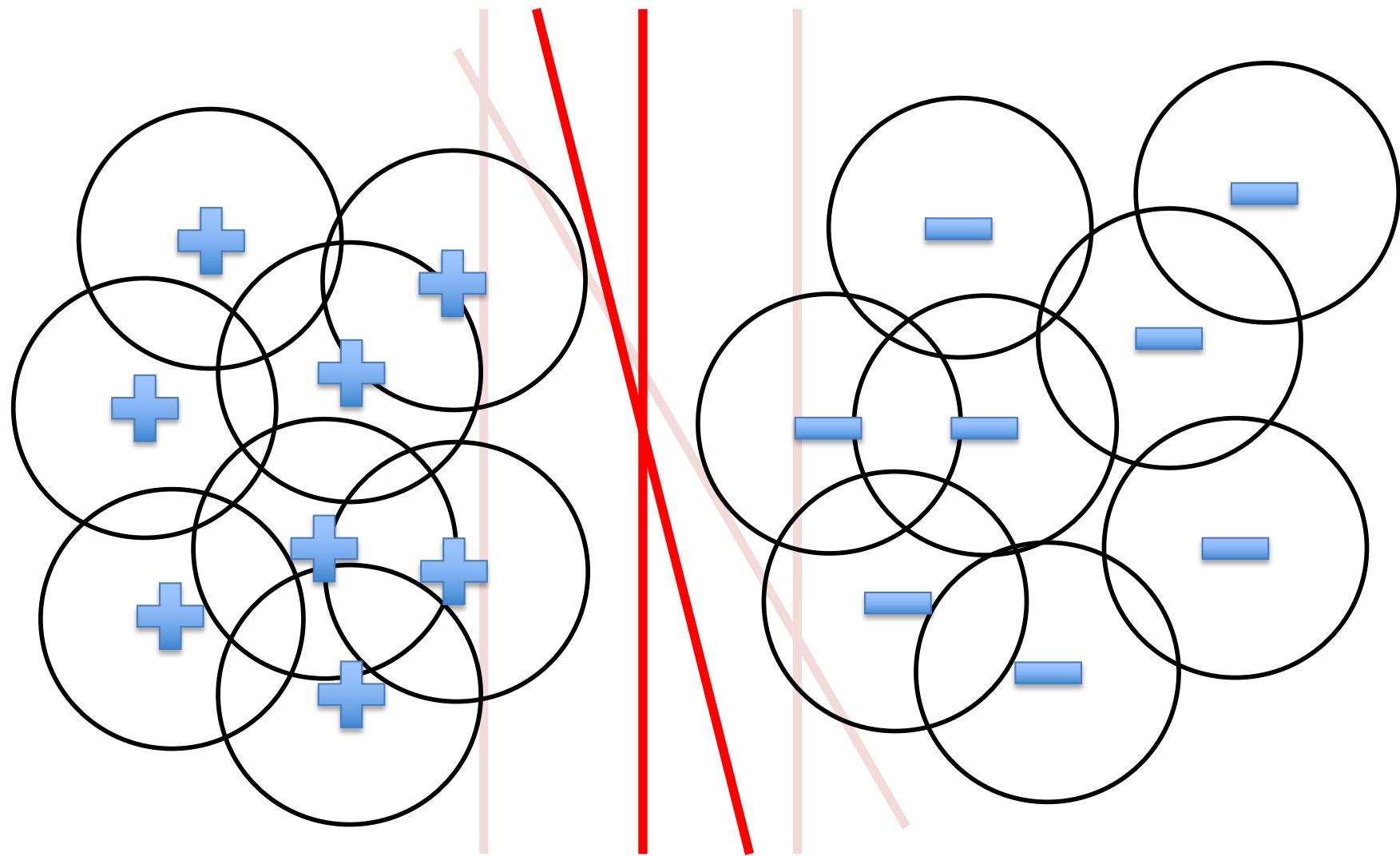
# Noise in the Observations



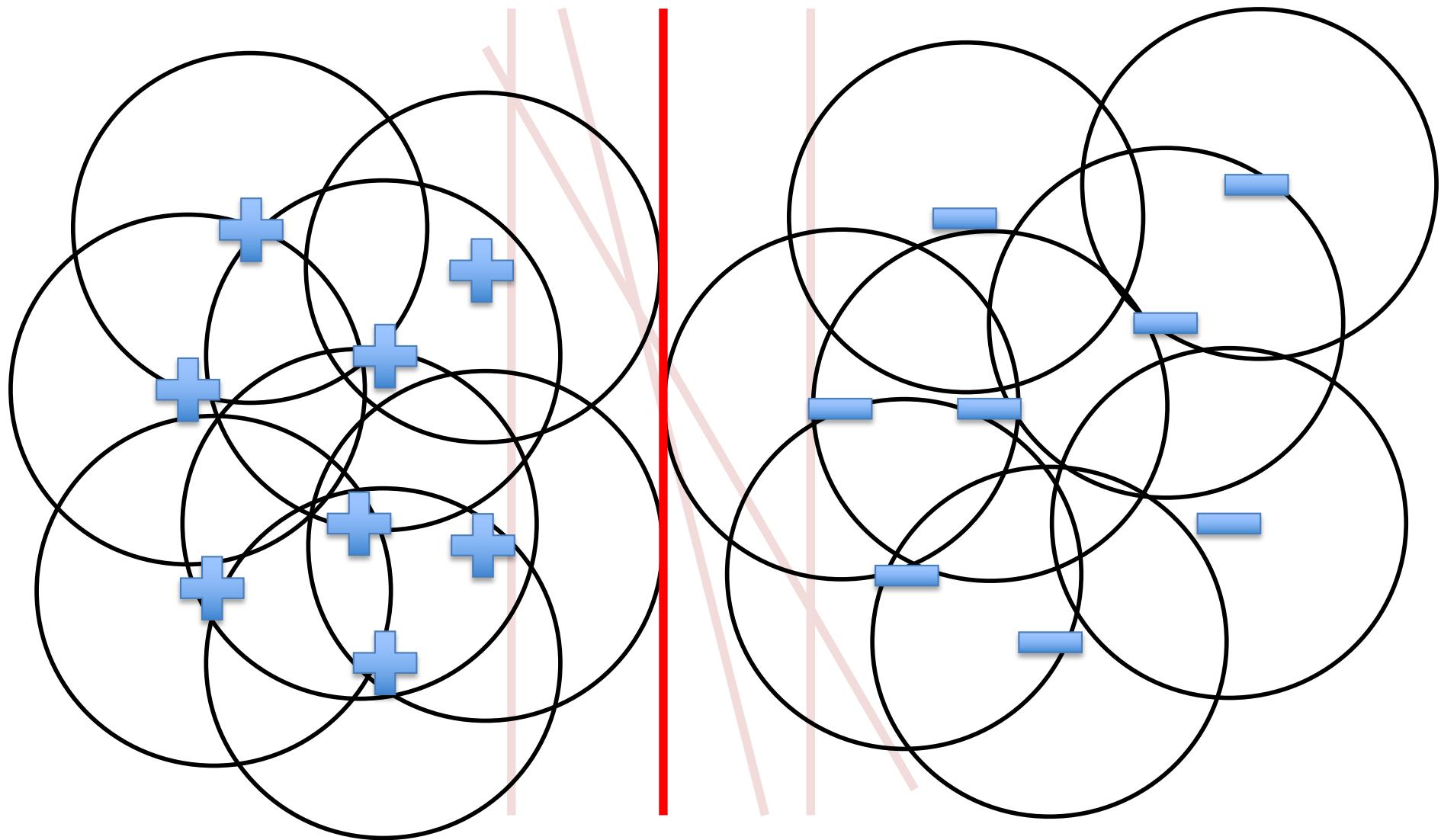
# Ruling Out Some Separators



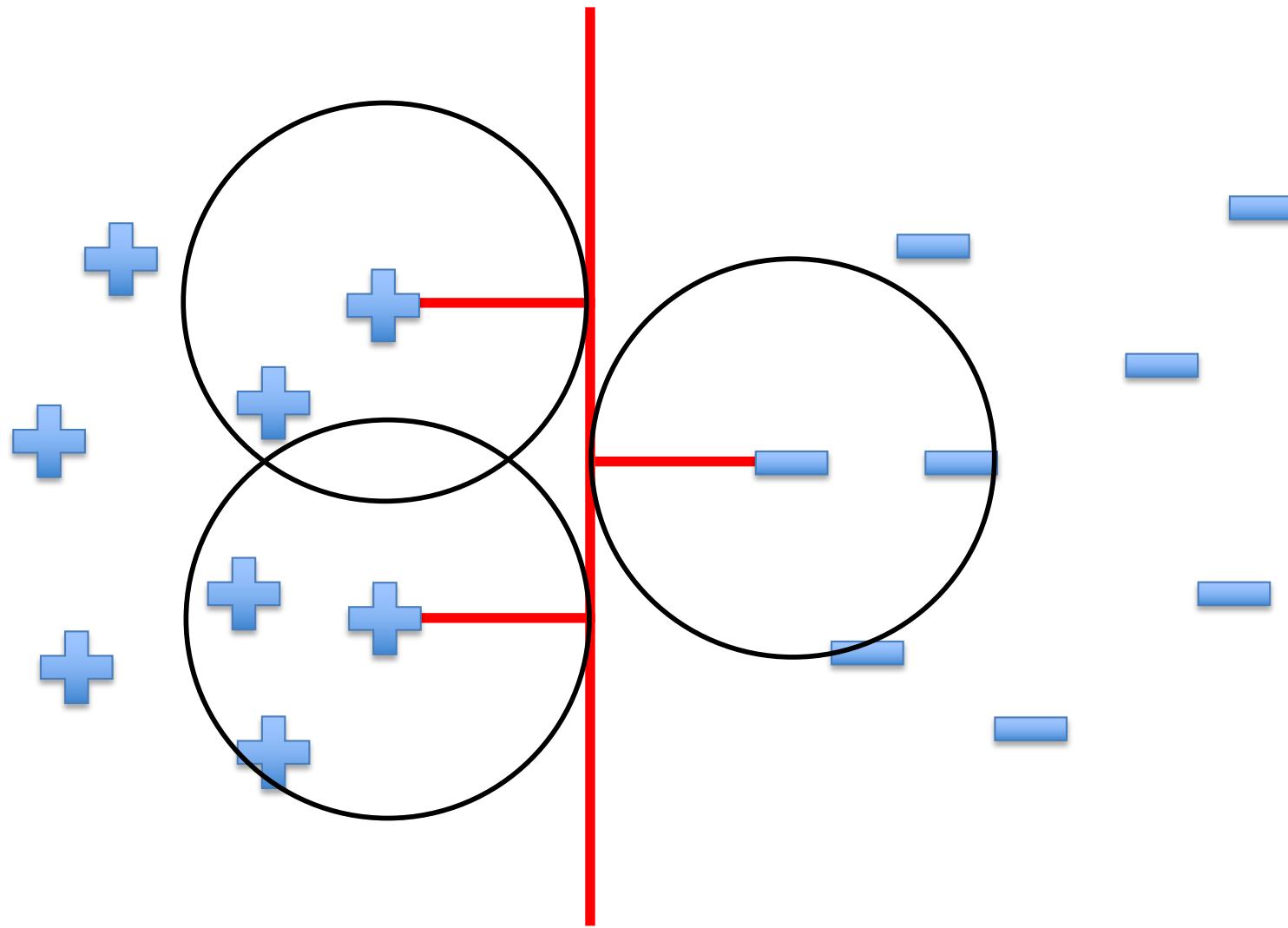
# Lots of Noise



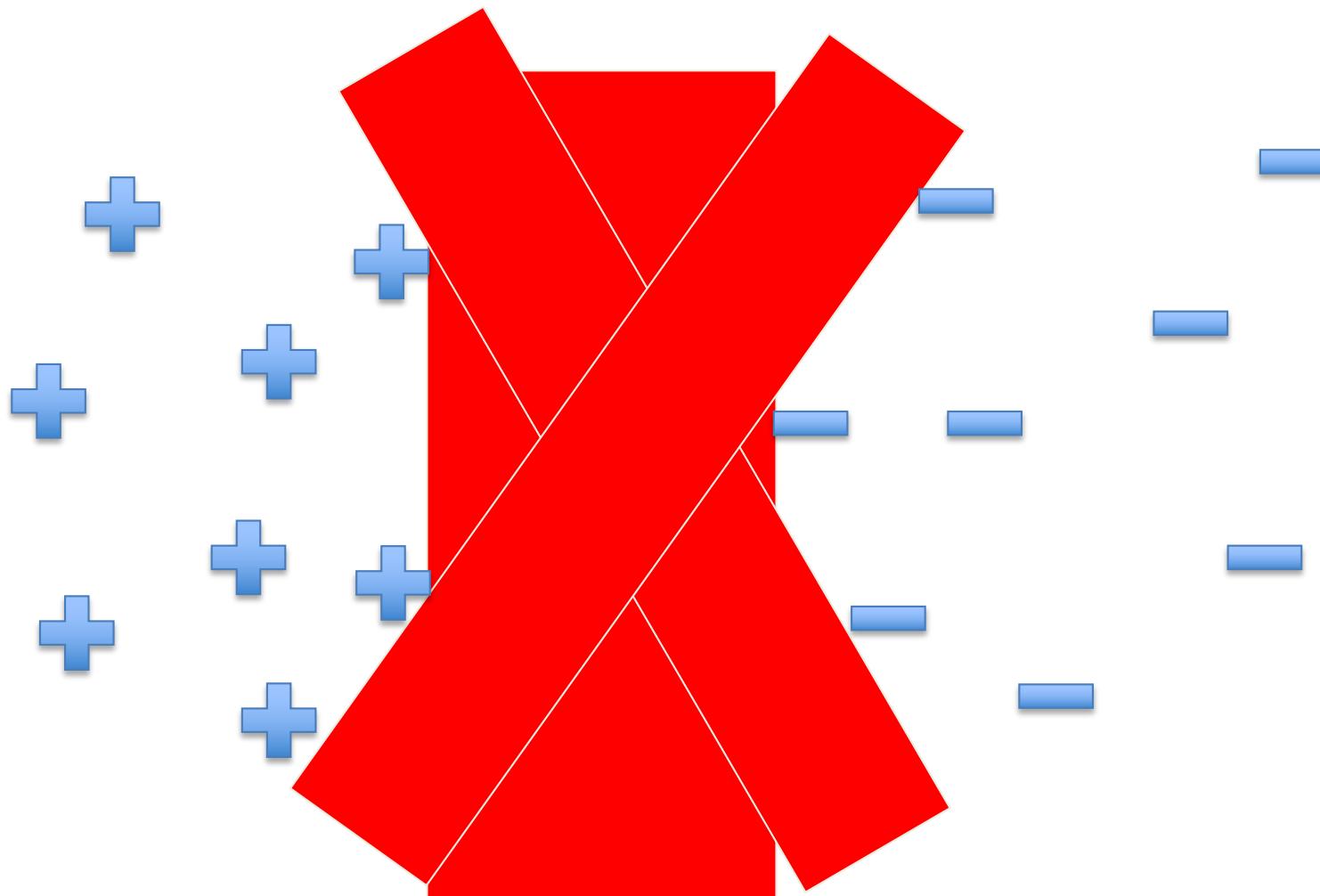
# Only One Separator Remains



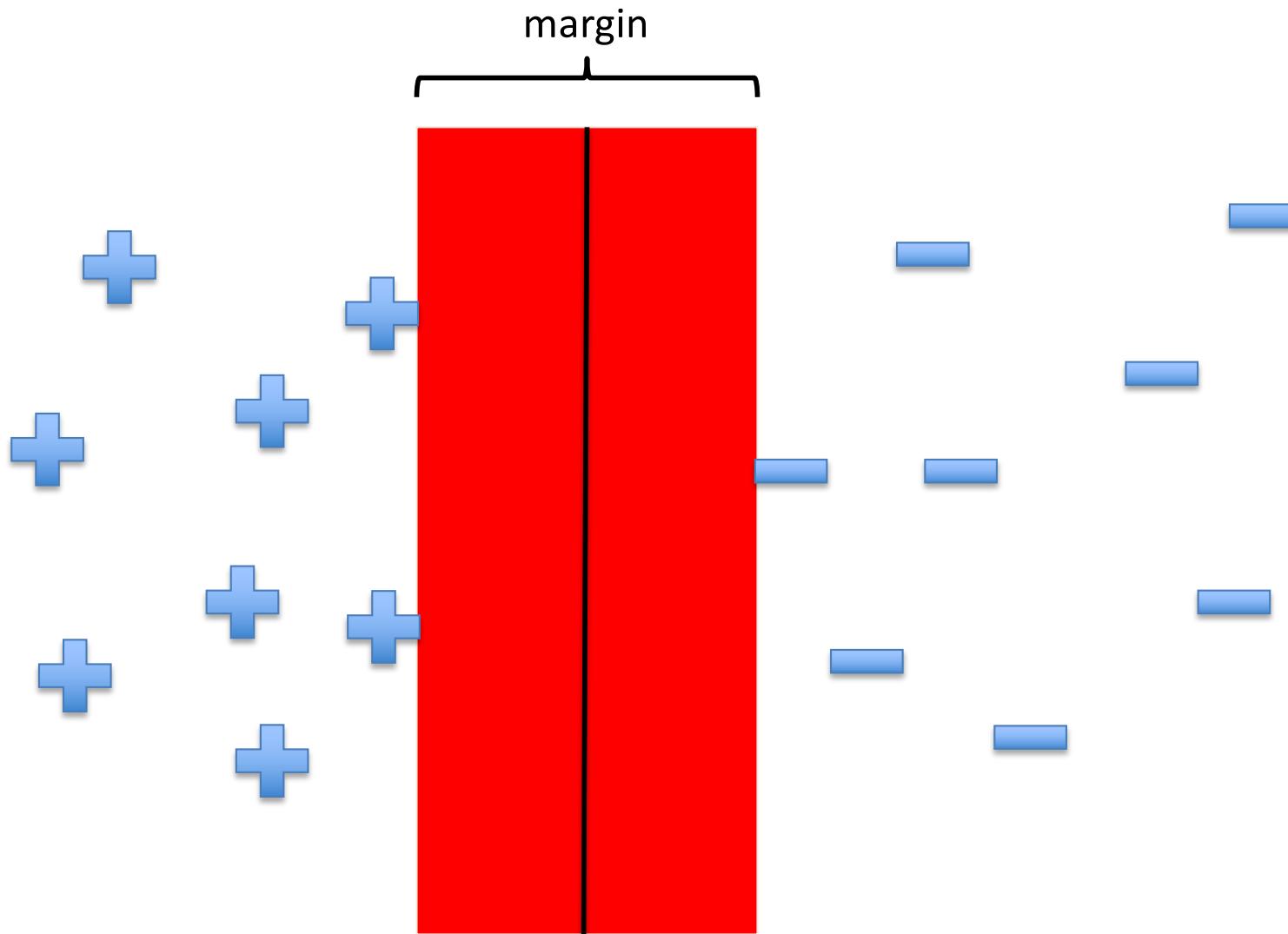
# Maximizing the Margin



# “Fat” Separators



# “Fat” Separators



# Why Maximize Margin

Increasing margin reduces *capacity*

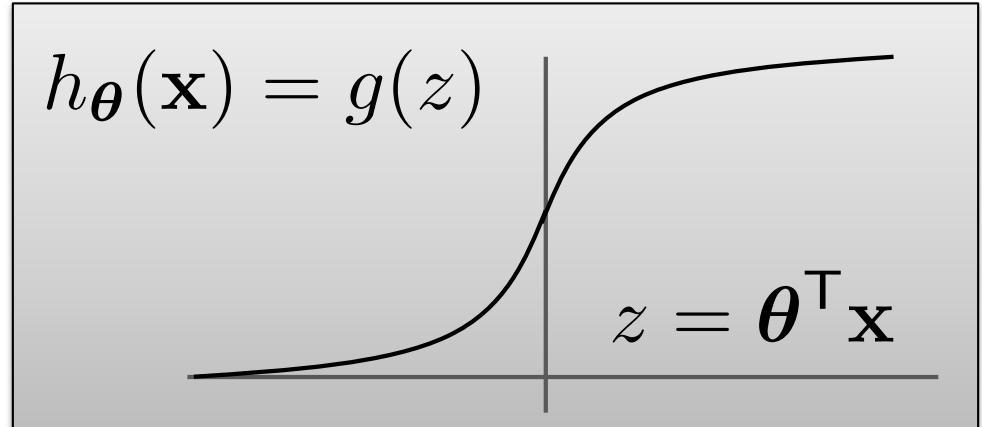
- i.e., fewer possible models

Lesson from Learning Theory:

- If the following holds:
  - $H$  is sufficiently constrained in size
  - and/or the size of the training data set  $n$  is large, then low training error is likely to be evidence of low generalization error

# Alternative View of Logistic Regression

$$h_{\theta}(\mathbf{x}) = \frac{1}{1 + e^{-\theta^T \mathbf{x}}}$$



The Logistic Regression Objective Function:

$$J(\theta) = - \sum_{i=1}^n [y_i \log h_{\theta}(\mathbf{x}_i) + (1 - y_i) \log (1 - h_{\theta}(\mathbf{x}_i))]$$
$$\min_{\theta} J(\theta) \quad \underbrace{\text{cost}_1(\theta^T \mathbf{x}_i)} \quad \underbrace{\text{cost}_0(\theta^T \mathbf{x}_i)}$$

Intuition: If  $y = 1$ , we want  $h_{\theta}(\mathbf{x}) \approx 1$ ,  $\theta^T \mathbf{x} \gg 0$

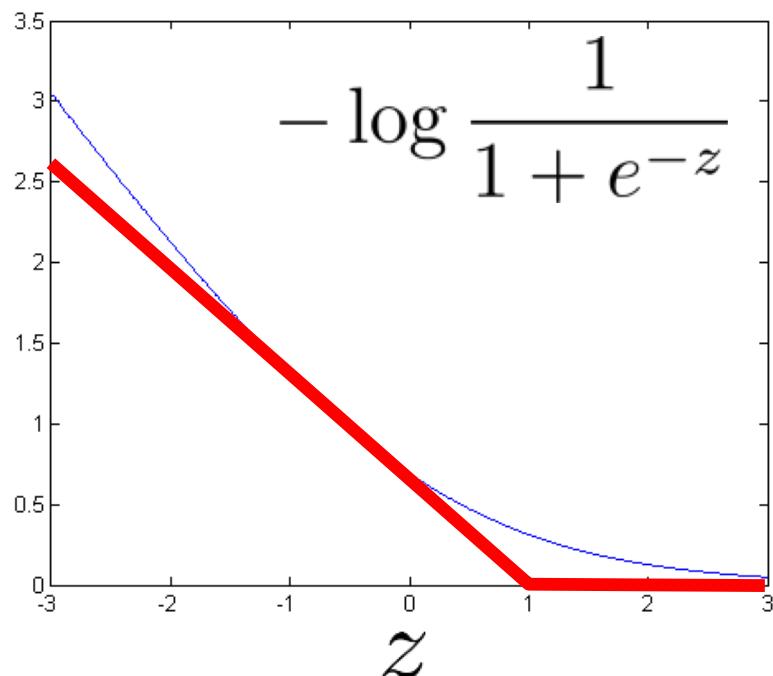
If  $y = 0$ , we want  $h_{\theta}(\mathbf{x}) \approx 0$ ,  $\theta^T \mathbf{x} \ll 0$

# Alternate View of Logistic Regression

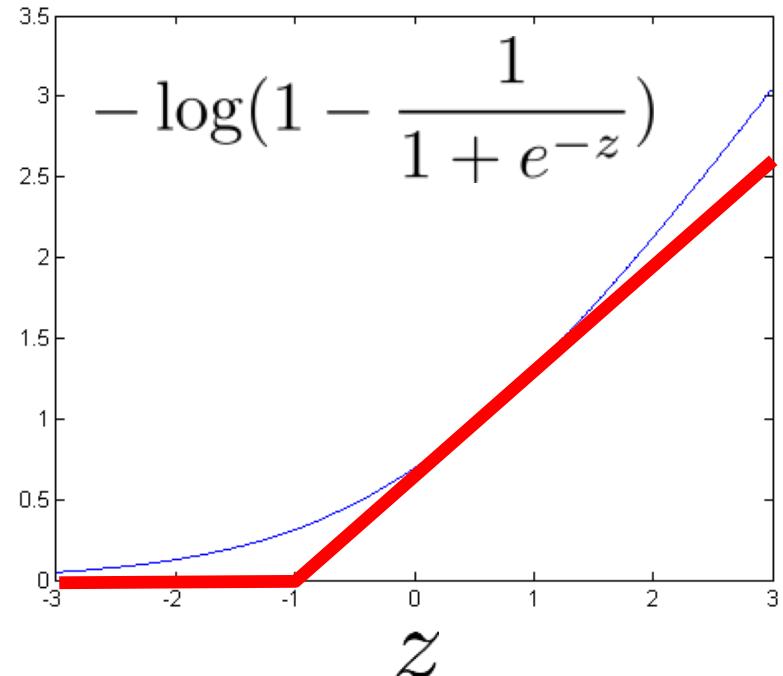
Cost of example:  $-y_i \log h_{\theta}(\mathbf{x}_i) - (1 - y_i) \log (1 - h_{\theta}(\mathbf{x}_i))$

$$h_{\theta}(\mathbf{x}) = \frac{1}{1 + e^{-\theta^T \mathbf{x}}} \quad z = \theta^T \mathbf{x}$$

If  $y = 1$  (want  $\theta^T \mathbf{x} \gg 0$ ):



If  $y = 0$  (want  $\theta^T \mathbf{x} \ll 0$ ):



# Logistic Regression to SVMs

Logistic Regression:

$$\min_{\theta} -\sum_{i=1}^n [y_i \log h_{\theta}(\mathbf{x}_i) + (1 - y_i) \log (1 - h_{\theta}(\mathbf{x}_i))] + \frac{\lambda}{2} \sum_{j=1}^d \theta_j^2$$

Support Vector Machines:

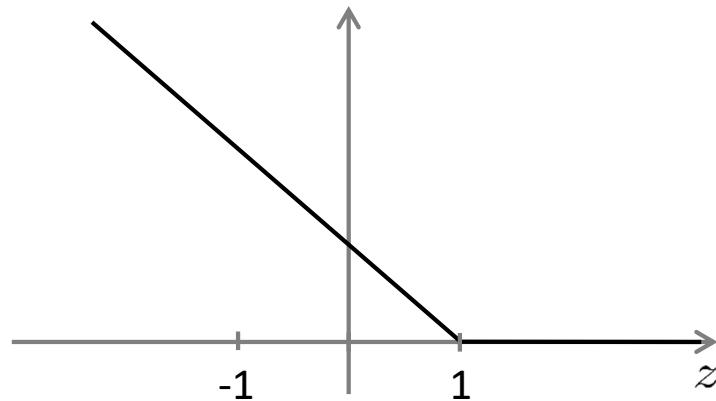
$$\min_{\theta} C \sum_{i=1}^n [y_i \text{cost}_1(\boldsymbol{\theta}^\top \mathbf{x}_i) + (1 - y_i) \text{cost}_0(\boldsymbol{\theta}^\top \mathbf{x}_i)] + \frac{1}{2} \sum_{j=1}^d \theta_j^2$$

You can think of  $C$  as similar to  $\frac{1}{\lambda}$

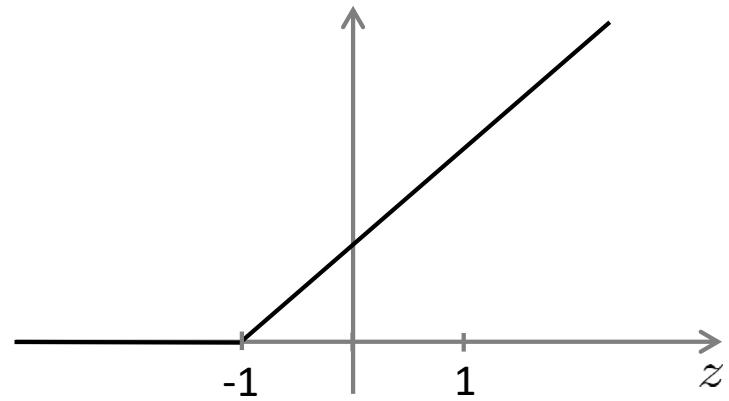
# Support Vector Machine

$$\min_{\theta} C \sum_{i=1}^n [y_i \text{cost}_1(\theta^\top \mathbf{x}_i) + (1 - y_i) \text{cost}_0(\theta^\top \mathbf{x}_i)] + \frac{1}{2} \sum_{j=1}^d \theta_j^2$$

If  $y = 1$  (want  $\theta^\top \mathbf{x} \geq 1$ ):



If  $y = 0$  (want  $\theta^\top \mathbf{x} \leq -1$ ):



$$\ell_{\text{hinge}}(h(\mathbf{x})) = \max(0, 1 - y \cdot h(\mathbf{x}))$$

# Support Vector Machine

$$\min_{\theta} C \sum_{i=1}^n [y_i \text{cost}_1(\boldsymbol{\theta}^\top \mathbf{x}_i) + (1 - y_i) \text{cost}_0(\boldsymbol{\theta}^\top \mathbf{x}_i)] + \frac{1}{2} \sum_{j=1}^d \theta_j^2$$

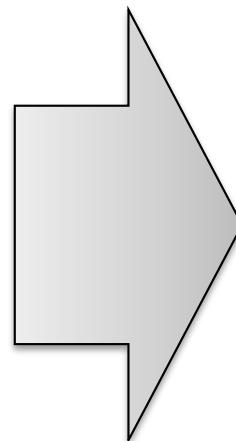
with  $C = 1$

$y = 1 / 0$

$y = +1 / -1$

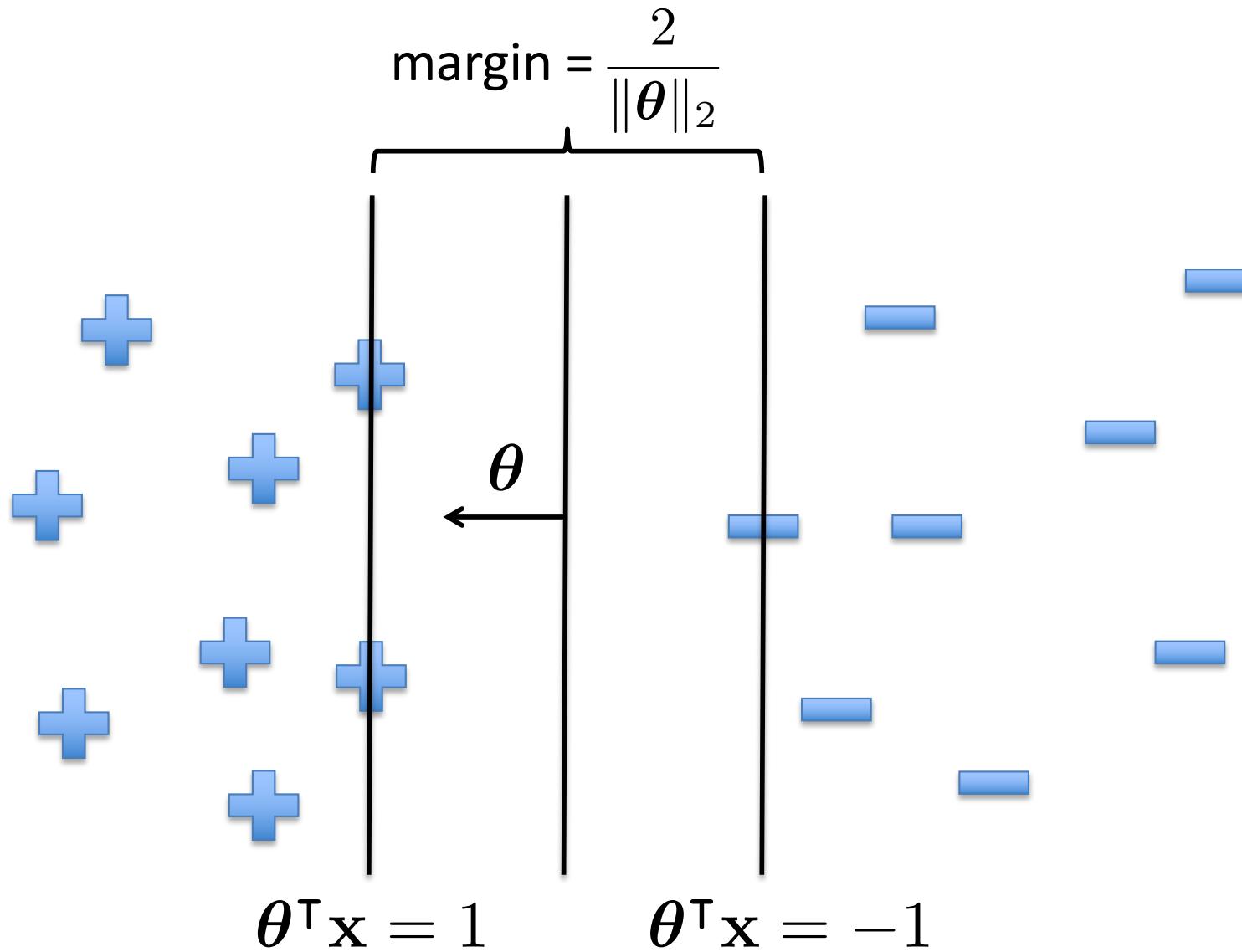
$$\min_{\theta} \frac{1}{2} \sum_{j=1}^d \theta_j^2$$

$$\begin{aligned} \text{s.t. } \boldsymbol{\theta}^\top \mathbf{x}_i &\geq 1 & \text{if } y_i = 1 \\ \boldsymbol{\theta}^\top \mathbf{x}_i &\leq -1 & \text{if } y_i = -1 \end{aligned}$$

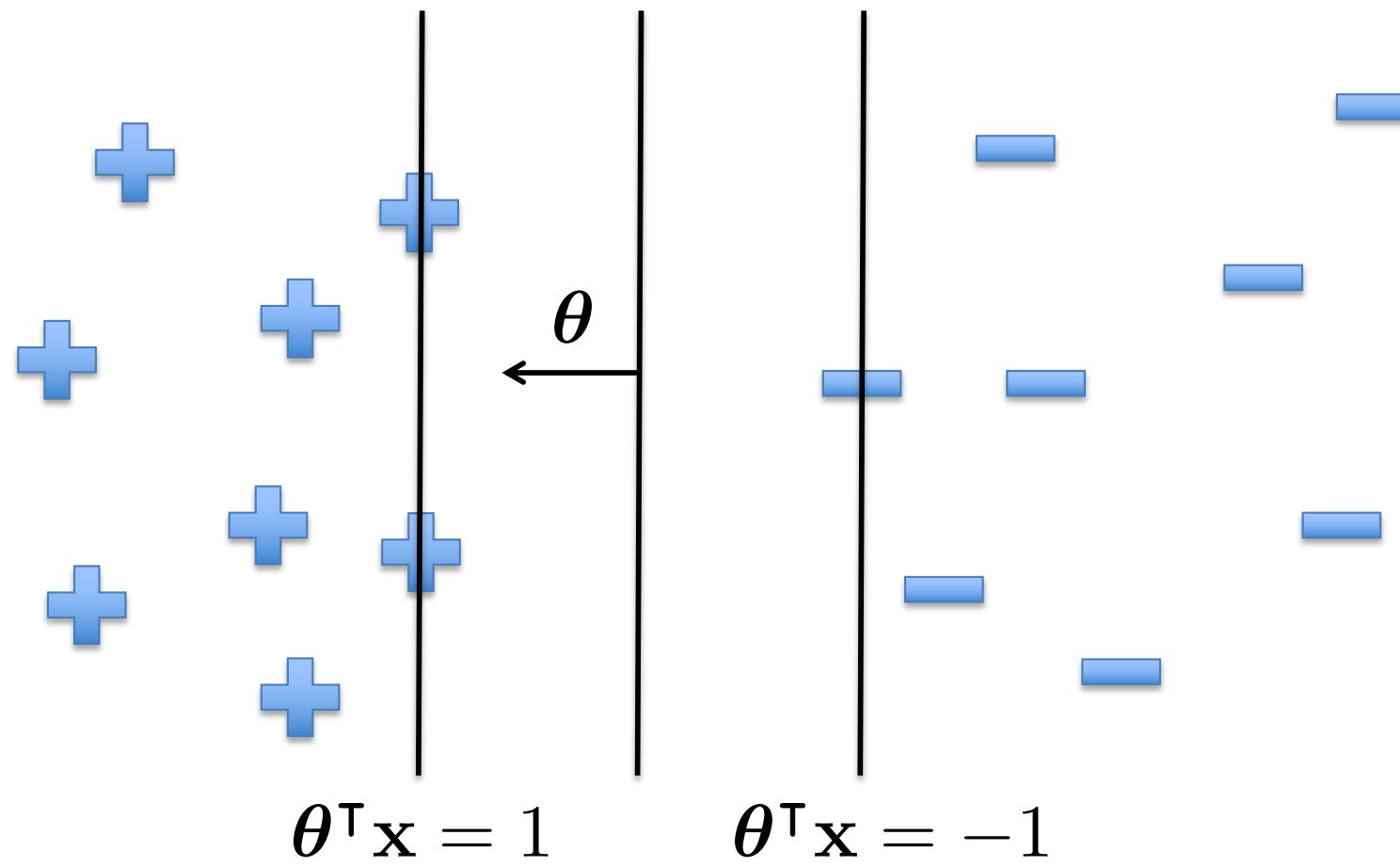


$$\begin{aligned} \min_{\theta} \frac{1}{2} \sum_{j=1}^d \theta_j^2 \\ \text{s.t. } y_i(\boldsymbol{\theta}^\top \mathbf{x}_i) &\geq 1 \end{aligned}$$

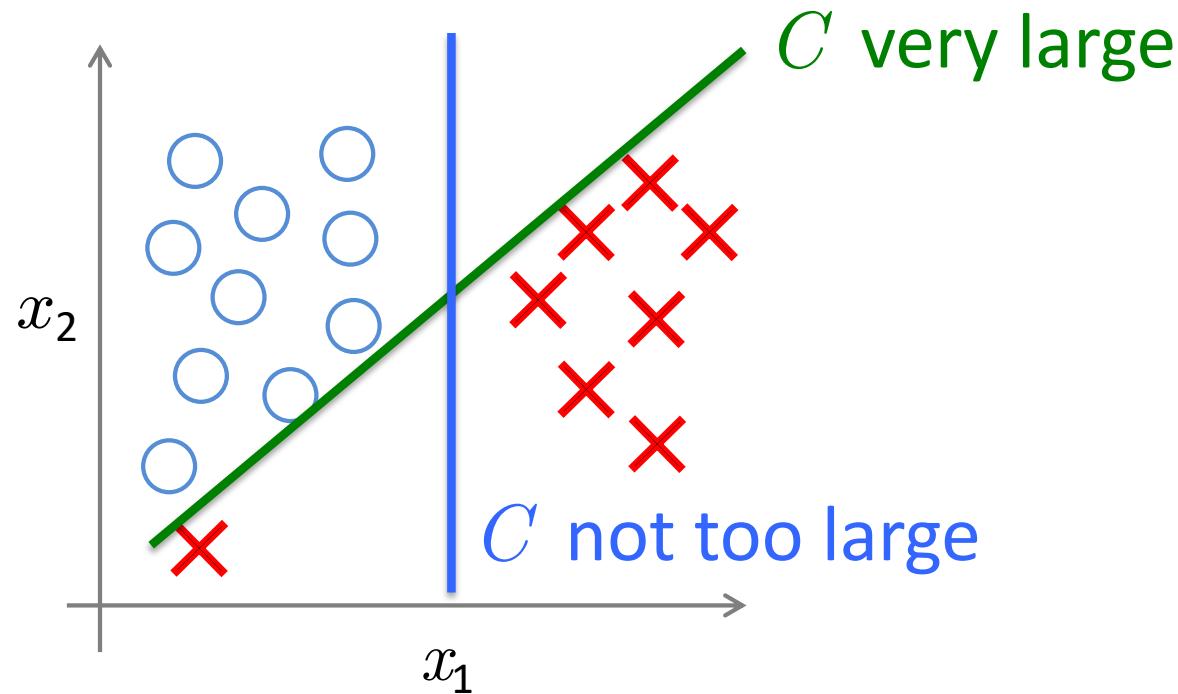
# Maximum Margin Hyperplane



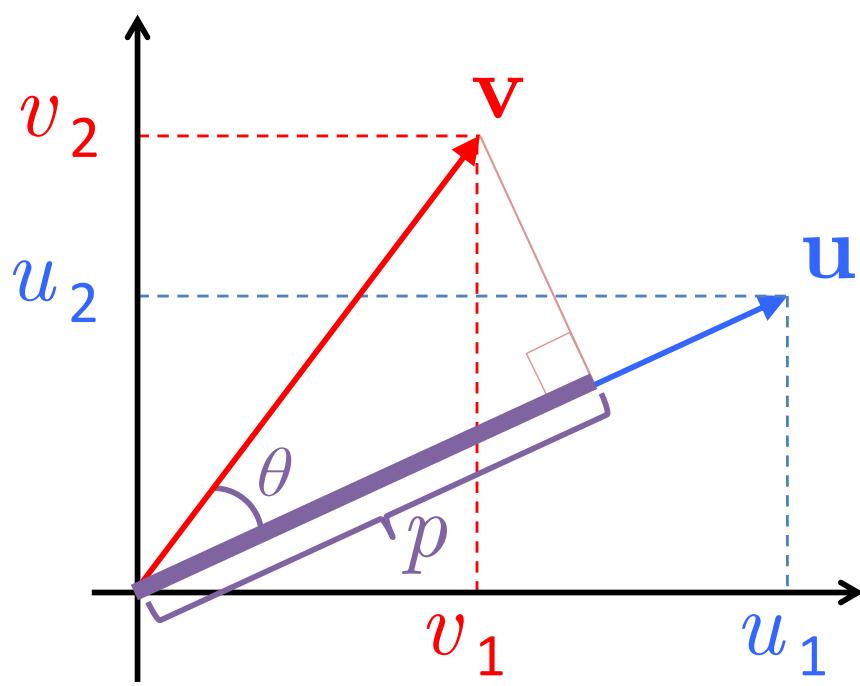
# Support Vectors



# Large Margin Classifier in Presence of Outliers



# Vector Inner Product



$$u = \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} \quad v = \begin{bmatrix} v_1 \\ v_2 \end{bmatrix}$$

$$\|\mathbf{u}\|_2 = \text{length}(\mathbf{u}) \in \mathbb{R}$$

$$= \sqrt{u_1^2 + u_2^2}$$

$$\mathbf{u}^\top \mathbf{v} = \mathbf{v}^\top \mathbf{u}$$

$$= u_1 v_1 + u_2 v_2$$

$$= \|\mathbf{u}\|_2 \|\mathbf{v}\|_2 \cos \theta$$

$$= p \|\mathbf{u}\|_2 \quad \text{where } p = \|\mathbf{v}\|_2 \cos \theta$$

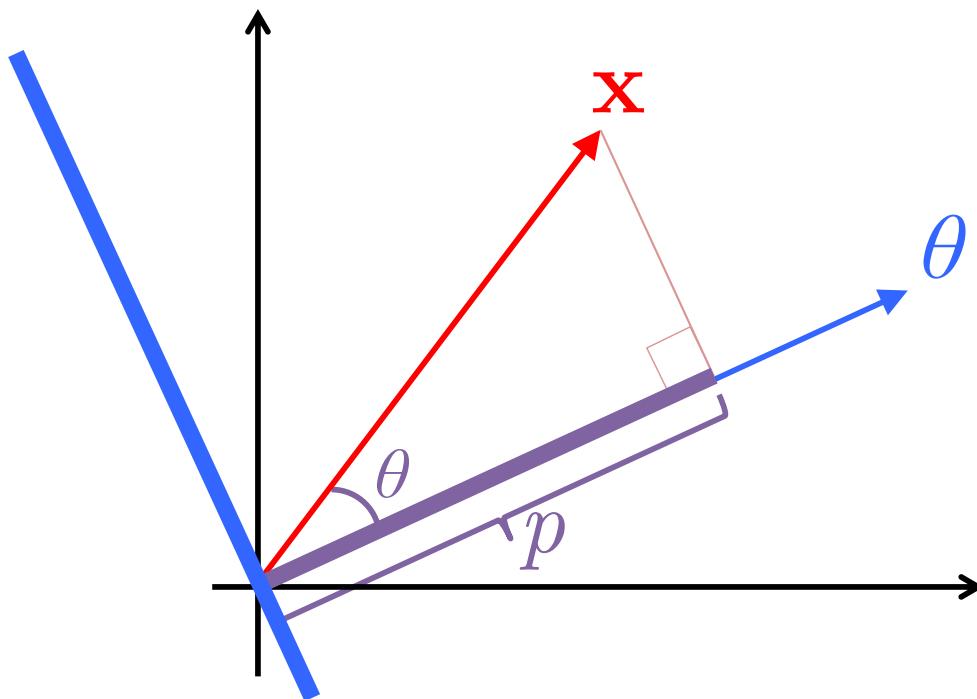
# Understanding the Hyperplane

$$\min_{\theta} \frac{1}{2} \sum_{j=1}^d \theta_j^2$$

s.t.  $\theta^\top \mathbf{x}_i \geq 1 \quad \text{if } y_i = 1$

$\theta^\top \mathbf{x}_i \leq -1 \quad \text{if } y_i = -1$

Assume  $\theta_0 = 0$  so that the hyperplane is centered at the origin, and that  $d = 2$



$$\begin{aligned}\theta^\top \mathbf{x} &= \|\theta\|_2 \underbrace{\|\mathbf{x}\|_2 \cos \theta}_p \\ &= p \|\theta\|_2\end{aligned}$$

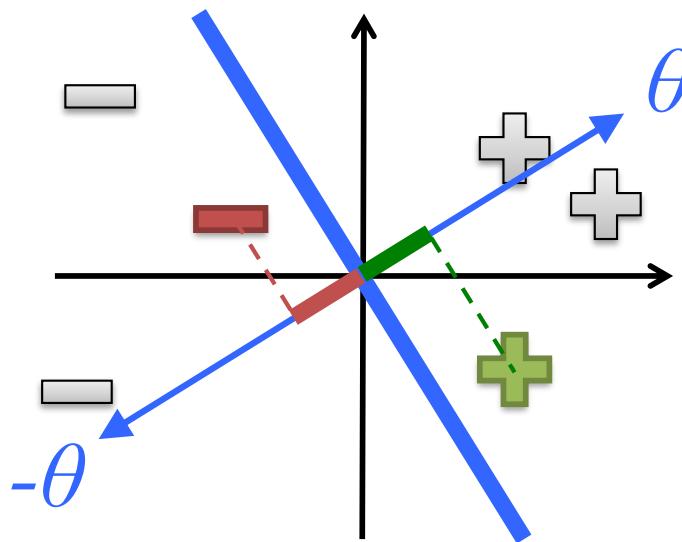
# Maximizing the Margin

$$\min_{\theta} \frac{1}{2} \sum_{j=1}^d \theta_j^2$$

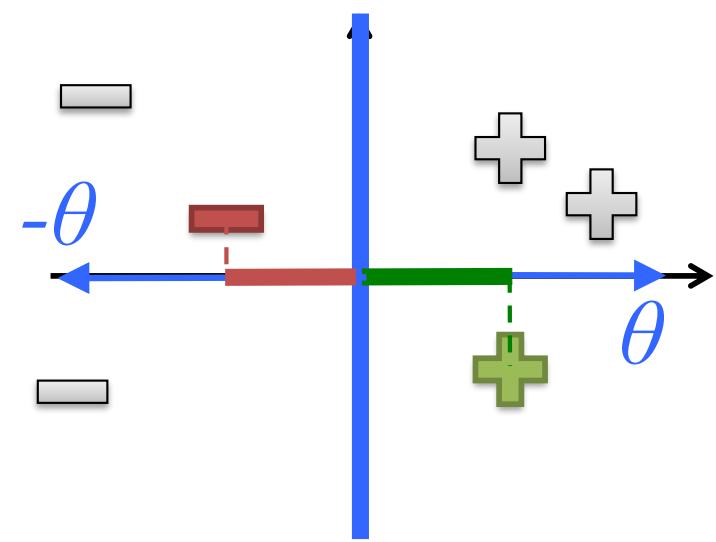
s.t.  $\theta^\top \mathbf{x}_i \geq 1 \quad \text{if } y_i = 1$   
 $\theta^\top \mathbf{x}_i \leq -1 \quad \text{if } y_i = -1$

Assume  $\theta_0 = 0$  so that the hyperplane is centered at the origin, and that  $d = 2$

Let  $p_i$  be the projection of  $\mathbf{x}_i$  onto the vector  $\theta$



Since  $p$  is small, therefore  $\|\theta\|_2$  must be large to have  $p\|\theta\|_2 \geq 1$  (or  $\leq -1$ )

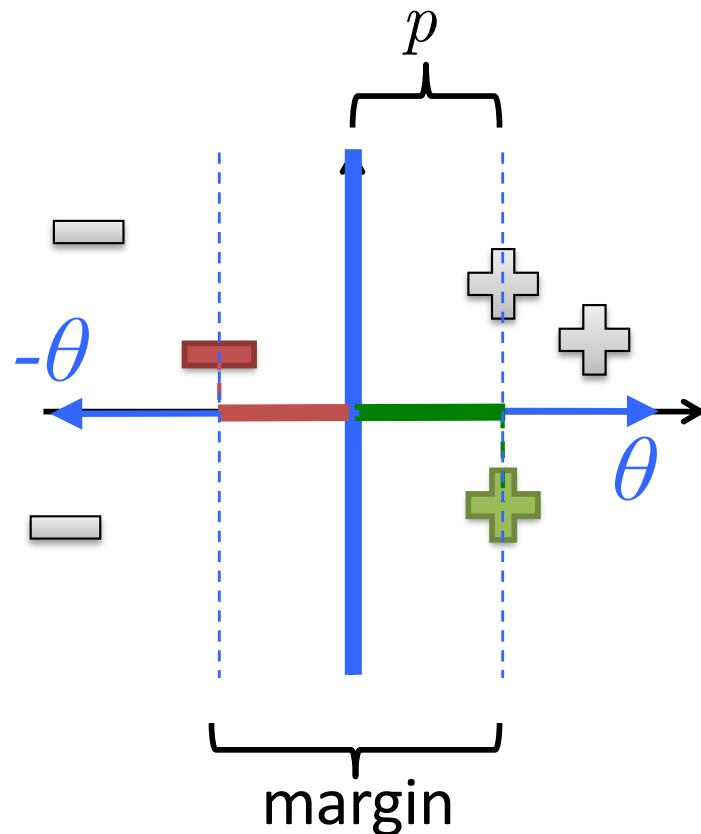


Since  $p$  is larger,  $\|\theta\|_2$  can be smaller in order to have  $p\|\theta\|_2 \geq 1$  (or  $\leq -1$ )

# Size of the Margin

For the support vectors, we have  $p\|\theta\|_2 = \pm 1$

- $p$  is the length of the projection of the SVs onto  $\theta$



Therefore,

$$p = \frac{1}{\|\theta\|_2}$$

$$\text{margin} = 2p = \frac{2}{\|\theta\|_2}$$

# The SVM Dual Problem

The primal SVM problem was given as

$$\begin{aligned} \min_{\theta} \quad & \frac{1}{2} \sum_{j=1}^d \theta_j^2 \\ \text{s.t.} \quad & y_i(\boldsymbol{\theta}^\top \mathbf{x}_i) \geq 1 \quad \forall i \end{aligned}$$

Can solve it more efficiently by taking the Lagrangian dual

- Duality is a common idea in optimization
- It transforms a difficult optimization problem into a simpler one
- Key idea: introduce slack variables  $\alpha_i$  for each constraint
  - $\alpha_i$  indicates how important a particular constraint is to the solution

# The SVM Dual Problem

- The Lagrangian is given by

$$L(\theta, \alpha) = \frac{1}{2} \sum_{j=1}^d \theta_j^2 - \sum_{i=1}^n \alpha_i (y_i \theta^\top \mathbf{x} - 1)$$

s.t.  $\alpha_i \geq 0 \quad \forall i$

- We must minimize over  $\theta$  and maximize over  $\alpha$
- At optimal solution, partials w.r.t  $\theta$ 's are 0

Solve by a bunch of algebra and calculus ...  
and we obtain ...

# SVM Dual Representation

$$\text{Maximize } J(\alpha) = \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j y_i y_j \langle \mathbf{x}_i, \mathbf{x}_j \rangle$$

$$\text{s.t. } \alpha_i \geq 0 \quad \forall i$$

$$\sum_i \alpha_i y_i = 0$$

The decision function is given by

$$h(\mathbf{x}) = \text{sign} \left( \sum_{i \in \mathcal{SV}} \alpha_i y_i \langle \mathbf{x}, \mathbf{x}_i \rangle + b \right)$$

$$\text{where } b = \frac{1}{|\mathcal{SV}|} \sum_{i \in \mathcal{SV}} \left( y_i - \sum_{j \in \mathcal{SV}} \alpha_j y_j \langle \mathbf{x}_i, \mathbf{x}_j \rangle \right)$$

# Understanding the Dual

$$\text{Maximize } J(\alpha) = \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j y_i y_j \langle \mathbf{x}_i, \mathbf{x}_j \rangle$$

$$\text{s.t. } \alpha_i \geq 0 \quad \forall i$$

$$\sum_i \alpha_i y_i = 0$$

Balances between the weight of constraints for different classes

Constraint weights ( $\alpha_i$ 's) cannot be negative

# Understanding the Dual

$$\text{Maximize } J(\alpha) = \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j y_i y_j \langle \mathbf{x}_i, \mathbf{x}_j \rangle$$

$$\text{s.t. } \alpha_i \geq 0 \quad \forall i$$

$$\sum \alpha_i y_i < 0$$

Points with different labels increase the sum

Points with same label decrease the sum

Measures the similarity between points

Intuitively, we should be more careful around points near the margin

# Understanding the Dual

$$\text{Maximize } J(\alpha) = \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j y_i y_j \langle \mathbf{x}_i, \mathbf{x}_j \rangle$$

$$\text{s.t. } \alpha_i \geq 0 \quad \forall i$$

$$\sum_i \alpha_i y_i = 0$$

In the solution, either:

- $\alpha_i > 0$  and the constraint is tight ( $y_i(\theta^\top \mathbf{x}_i) = 1$ )
  - point is a support vector
- $\alpha_i = 0$ 
  - point is not a support vector

# Employing the Solution

- Given the optimal solution  $\alpha^*$ , optimal weights are

$$\theta^* = \sum_{i \in SVs} \alpha_i^* y_i \mathbf{x}_i$$

- In this formulation, have *not* added  $x_0 = 1$

- Therefore, we can solve one of the SV constraints

$$y_i(\theta^* \cdot \mathbf{x}_i + \theta_0) = 1$$

- to obtain  $\theta_0$

- Or, more commonly, take the average solution over all support vectors

# What if Data Are Not Linearly Separable?

- Cannot find  $\theta$  that satisfies  $y_i(\theta^\top \mathbf{x}_i) \geq 1 \quad \forall i$

- Introduce slack variables  $\xi_i$

$$y_i(\theta^\top \mathbf{x}_i) \geq 1 - \xi_i \quad \forall i$$

- New problem:

$$\min_{\theta} \frac{1}{2} \sum_{j=1}^d \theta_j^2 + C \sum_i \xi_i$$

$$\text{s.t. } y_i(\theta^\top \mathbf{x}_i) \geq 1 - \xi_i \quad \forall i$$

# Strengths of SVMs

- Good generalization in theory
- Good generalization in practice
- Work well with few training instances
- Find globally best model
- Efficient algorithms
- Amenable to the kernel trick ...

# What if Surface is Non-Linear?

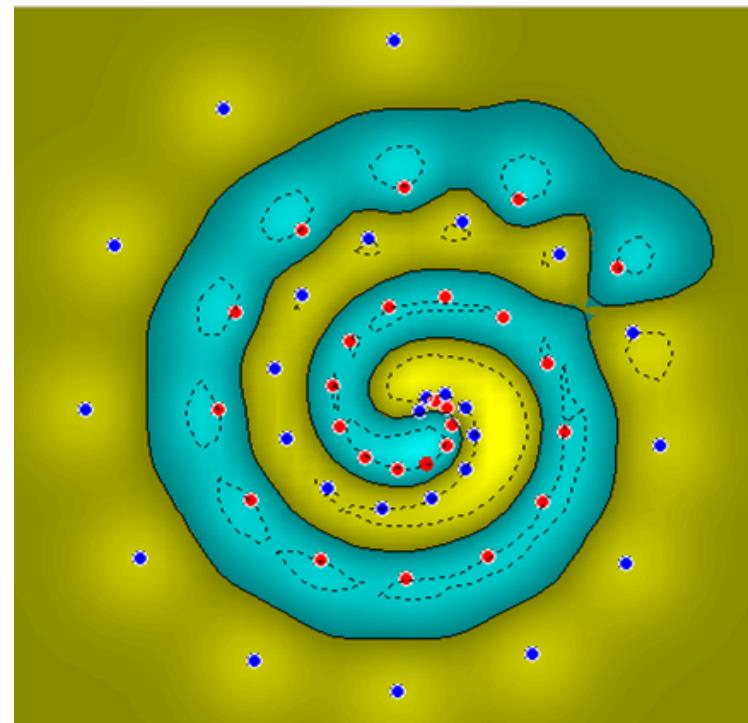
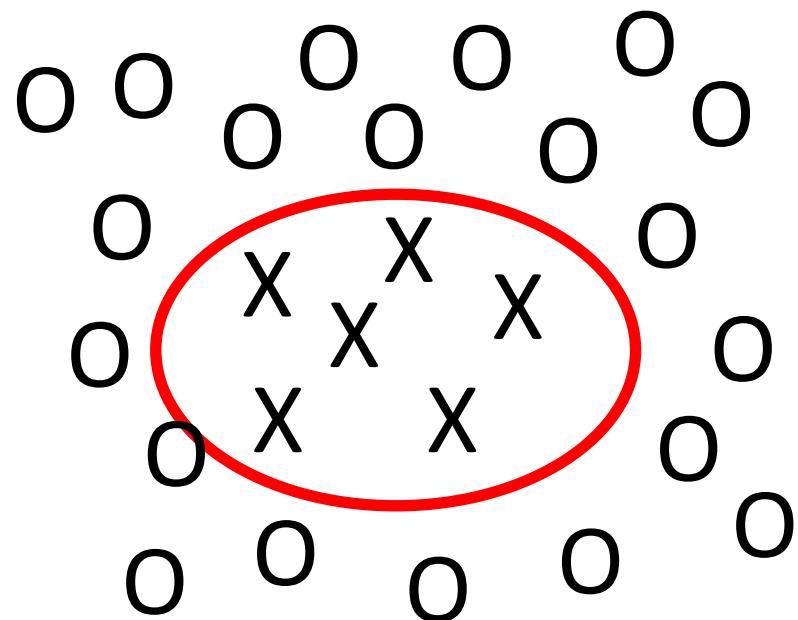
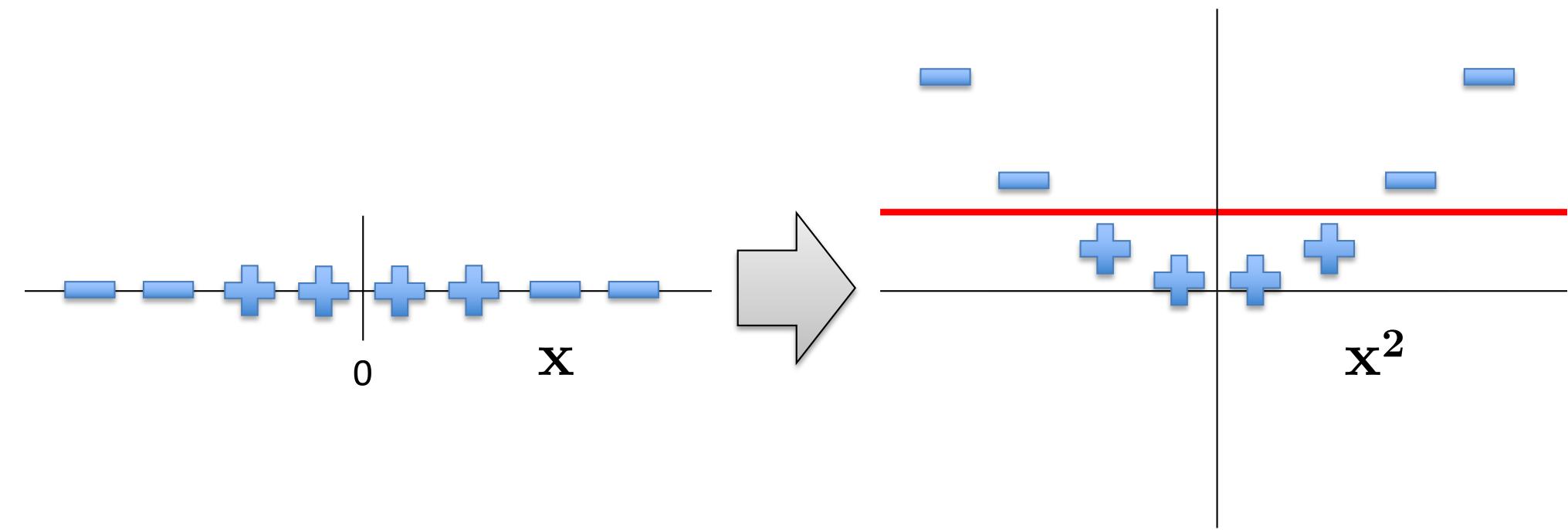


Image from <http://www.atrandomresearch.com/iclass/>

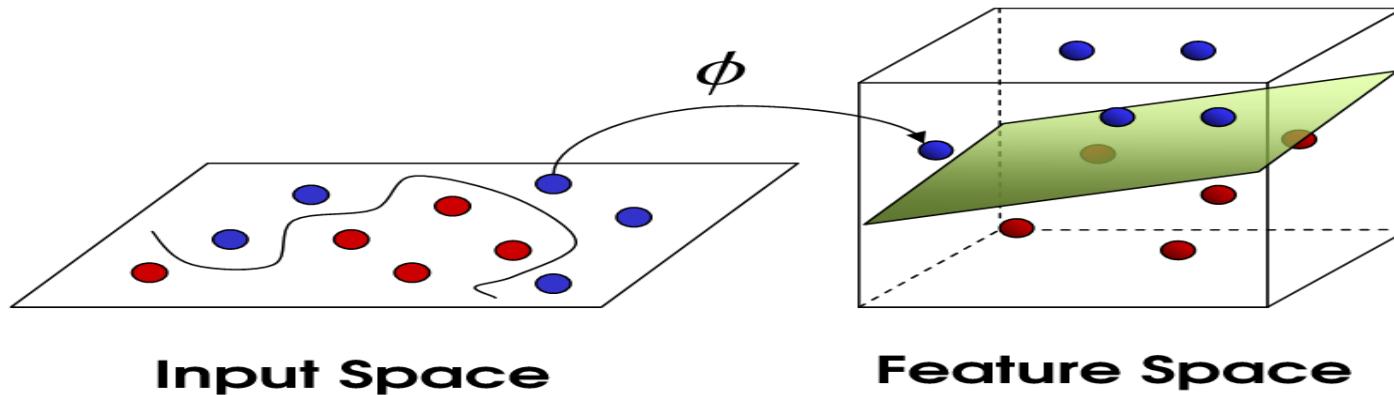
# Kernel Methods

Making the Non-Linear Linear

# When Linear Separators Fail



# Mapping into a New Feature Space



$$\Phi : \mathcal{X} \mapsto \hat{\mathcal{X}} = \Phi(\mathbf{x})$$

- For example, with  $\mathbf{x}_i \in \mathbb{R}^2$   
$$\Phi([x_{i1}, x_{i2}]) = [x_{i1}, x_{i2}, x_{i1}x_{i2}, x_{i1}^2, x_{i2}^2]$$
- Rather than run SVM on  $\mathbf{x}_i$ , run it on  $\Phi(\mathbf{x}_i)$ 
  - Find non-linear separator in input space
- What if  $\Phi(\mathbf{x}_i)$  is really big?
- Use kernels to compute it implicitly!

# Kernels

- Find kernel  $K$  such that

$$K(\mathbf{x}_i, \mathbf{x}_j) = \langle \Phi(\mathbf{x}_i), \Phi(\mathbf{x}_j) \rangle$$

- Computing  $K(\mathbf{x}_i, \mathbf{x}_j)$  should be efficient, much more so than computing  $\Phi(\mathbf{x}_i)$  and  $\Phi(\mathbf{x}_j)$
- Use  $K(\mathbf{x}_i, \mathbf{x}_j)$  in SVM algorithm rather than  $\langle \mathbf{x}_i, \mathbf{x}_j \rangle$
- Remarkably, this is possible!

# The Polynomial Kernel

Let  $\mathbf{x}_i = [x_{i1}, x_{i2}]$  and  $\mathbf{x}_j = [x_{j1}, x_{j2}]$

Consider the following function:

$$\begin{aligned} K(\mathbf{x}_i, \mathbf{x}_j) &= \langle \mathbf{x}_i, \mathbf{x}_j \rangle^2 \\ &= (x_{i1}x_{j1} + x_{i2}x_{j2})^2 \\ &= (x_{i1}^2x_{j1}^2 + x_{i2}^2x_{j2}^2 + 2x_{i1}x_{i2}x_{j1}x_{j2}) \\ &= \langle \Phi(\mathbf{x}_i), \Phi(\mathbf{x}_j) \rangle \end{aligned}$$

where

$$\Phi(\mathbf{x}_i) = [x_{i1}^2, x_{i2}^2, \sqrt{2}x_{i1}x_{i2}]$$

$$\Phi(\mathbf{x}_j) = [x_{j1}^2, x_{j2}^2, \sqrt{2}x_{j1}x_{j2}]$$

# The Polynomial Kernel

- Given by  $K(\mathbf{x}_i, \mathbf{x}_j) = \langle \mathbf{x}_i, \mathbf{x}_j \rangle^d$ 
  - $\Phi(\mathbf{x})$  contains all monomials of degree  $d$
- Useful in visual pattern recognition
  - Example:
    - 16x16 pixel image
    - $10^{10}$  monomials of degree 5
    - Never explicitly compute  $\Phi(\mathbf{x})$  !
- Variation:  $K(\mathbf{x}_i, \mathbf{x}_j) = (\langle \mathbf{x}_i, \mathbf{x}_j \rangle + 1)^d$ 
  - Adds all lower-order monomials (degrees 1,..., $d$  )!

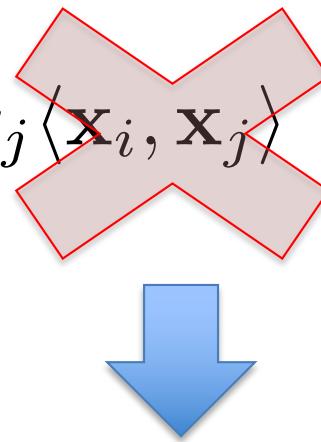
# The Kernel Trick

“Given an algorithm which is formulated in terms of a positive definite kernel  $K_1$ , one can construct an alternative algorithm by replacing  $K_1$  with another positive definite kernel  $K_2$ ”

- SVMs can use the kernel trick

# Incorporating Kernels into SVM

$$J(\alpha) = \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j y_i y_j \cancel{\langle \mathbf{x}_i, \mathbf{x}_j \rangle}$$



$$J(\alpha) = \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j y_i y_j K(\mathbf{x}_i, \mathbf{x}_j)$$

$$\text{s.t. } \alpha_i \geq 0 \quad \forall i$$

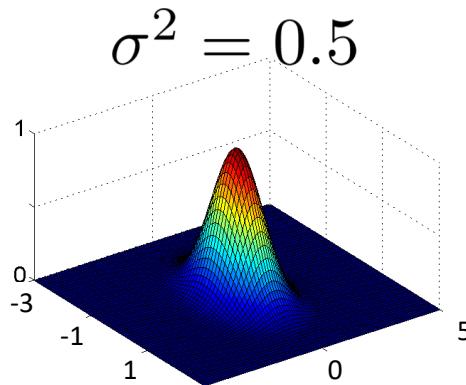
$$\sum_i \alpha_i y_i = 0$$

# The Gaussian Kernel

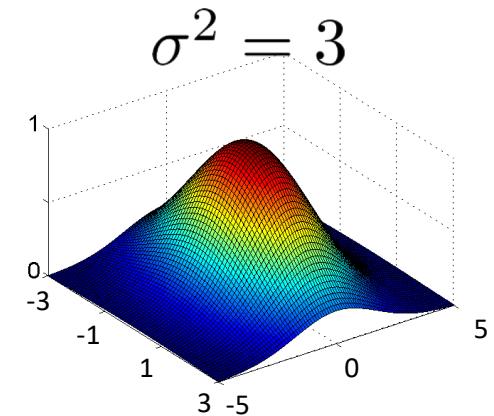
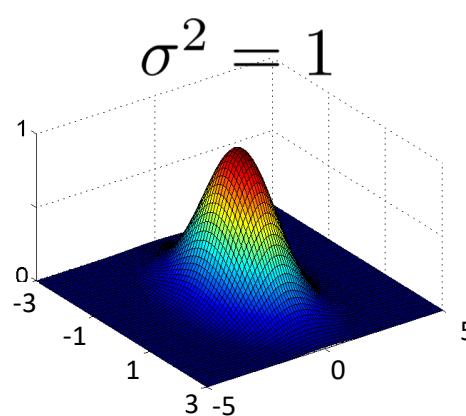
- Also called Radial Basis Function (RBF) kernel

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

- Has value 1 when  $\mathbf{x}_i = \mathbf{x}_j$
- Value falls off to 0 with increasing distance
- Note: Need to do feature scaling before using Gaussian Kernel



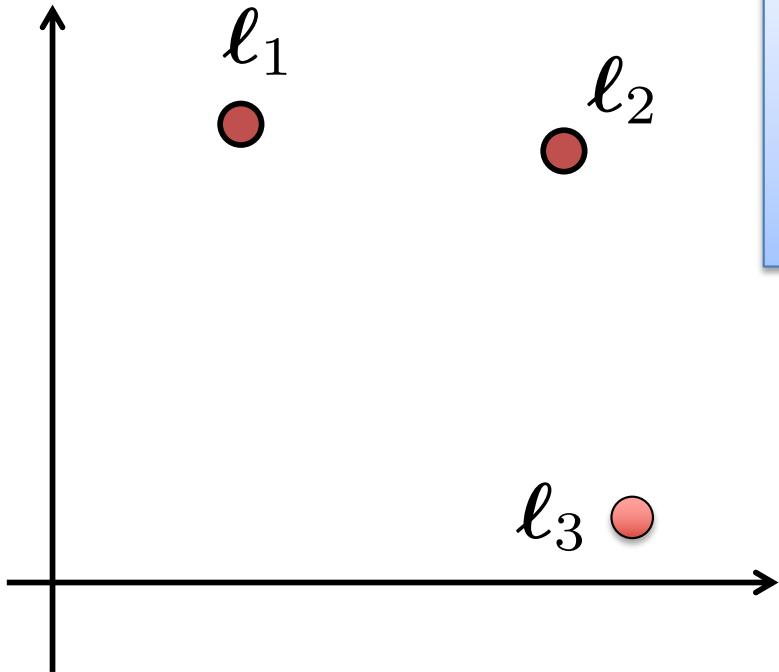
lower bias,  
higher variance



higher bias,  
lower variance



# Gaussian Kernel Example



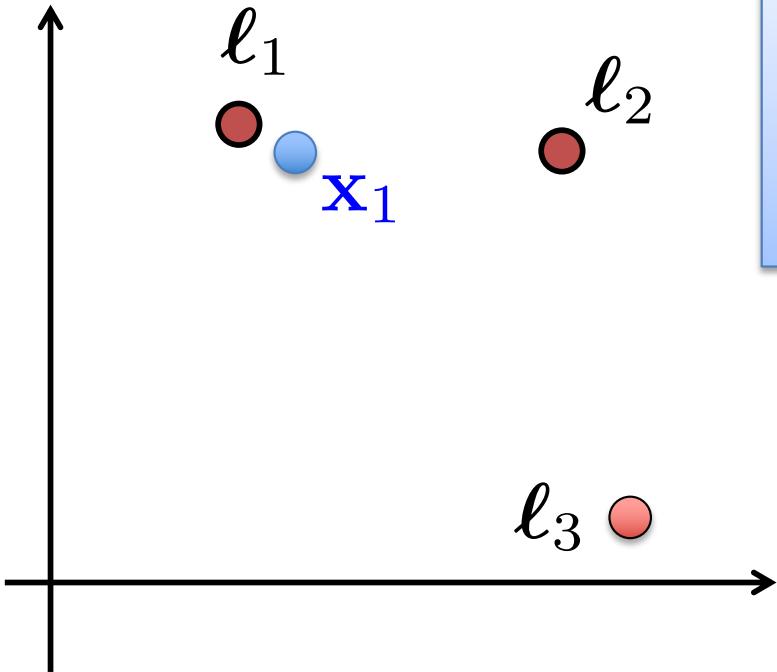
$$K(\mathbf{x}_i, \mathbf{x}_j) = \exp\left(-\frac{\|\mathbf{x}_i - \mathbf{x}_j\|_2^2}{2\sigma^2}\right)$$

Imagine we've learned that:

$$\theta = [-0.5, 1, 1, 0]$$

Predict +1 if  $\theta_0 + \theta_1 K(\mathbf{x}, \ell_1) + \theta_2 K(\mathbf{x}, \ell_2) + \theta_3 K(\mathbf{x}, \ell_3) \geq 0$

# Gaussian Kernel Example



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

Imagine we've learned that:

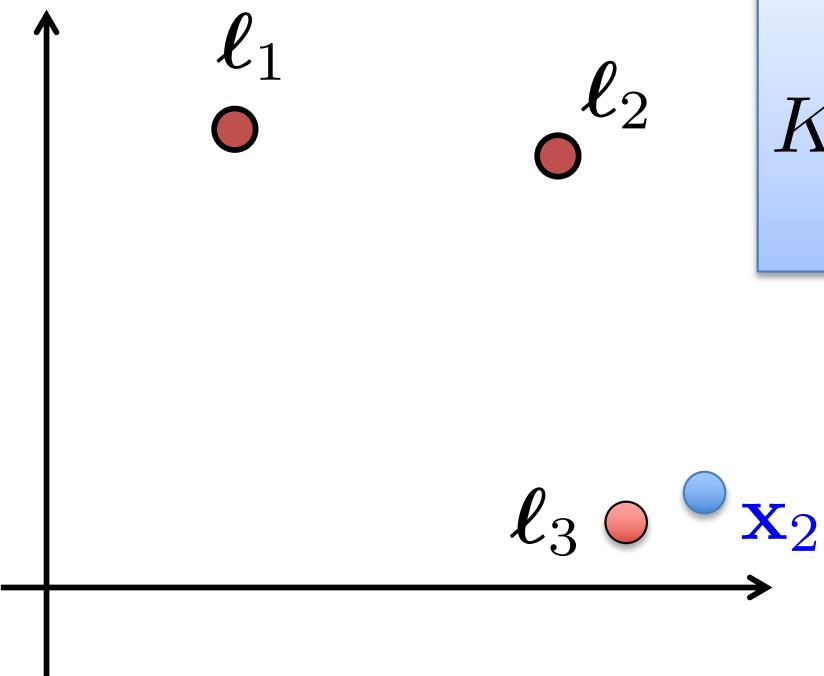
$$\theta = [-0.5, 1, 1, 0]$$

Predict +1 if  $\theta_0 + \theta_1 K(\mathbf{x}, \ell_1) + \theta_2 K(\mathbf{x}, \ell_2) + \theta_3 K(\mathbf{x}, \ell_3) \geq 0$

- For  $\mathbf{x}_1$ , we have  $K(\mathbf{x}_1, \ell_1) \approx 1$ , other similarities  $\approx 0$

$$\begin{aligned} & \theta_0 + \theta_1(1) + \theta_2(0) + \theta_3(0) \\ &= -0.5 + 1(1) + 1(0) + 0(0) \\ &= 0.5 \geq 0, \text{ so predict } +1 \end{aligned}$$

# Gaussian Kernel Example



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

Imagine we've learned that:

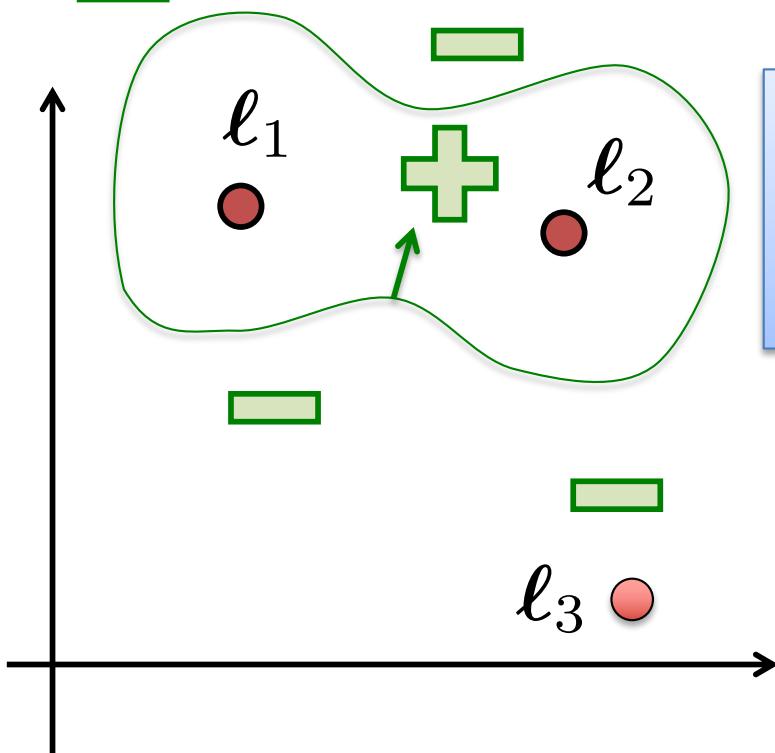
$$\theta = [-0.5, 1, 1, 0]$$

Predict +1 if  $\theta_0 + \theta_1 K(\mathbf{x}, \ell_1) + \theta_2 K(\mathbf{x}, \ell_2) + \theta_3 K(\mathbf{x}, \ell_3) \geq 0$

- For  $\mathbf{x}_2$ , we have  $K(\mathbf{x}_2, \ell_3) \approx 1$ , other similarities  $\approx 0$

$$\begin{aligned} & \theta_0 + \theta_1(0) + \theta_2(0) + \theta_3(1) \\ &= -0.5 + 1(0) + 1(0) + 0(1) \\ &= -0.5 < 0, \text{ so predict -1} \end{aligned}$$

# Gaussian Kernel Example



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

Imagine we've learned that:

$$\theta = [-0.5, 1, 1, 0]$$

Predict +1 if  $\theta_0 + \theta_1 K(\mathbf{x}, \ell_1) + \theta_2 K(\mathbf{x}, \ell_2) + \theta_3 K(\mathbf{x}, \ell_3) \geq 0$

Rough sketch of decision surface

# Other Kernels

- Sigmoid Kernel

$$K(\mathbf{x}_i, \mathbf{x}_j) = \tanh(\alpha \mathbf{x}_i^T \mathbf{x}_j + c)$$

- Neural networks use sigmoid as activation function
- SVM with a sigmoid kernel is equivalent to 2-layer perceptron

- Cosine Similarity Kernel

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

- Popular choice for measuring similarity of text documents
- L<sub>2</sub> norm projects vectors onto the unit sphere; their dot product is the cosine of the angle between the vectors

# Other Kernels

- Chi-squared Kernel

$$K(\mathbf{x}_i, \mathbf{x}_j) = \exp \left( -\gamma \sum_k \frac{(x_{ik} - x_{jk})^2}{x_{ik} + x_{jk}} \right)$$

- Widely used in computer vision applications
- Chi-squared measures distance between probability distributions
- Data is assumed to be non-negative, often with L<sub>1</sub> norm of 1

- String kernels
- Tree kernels
- Graph kernels

# An Aside: The Math Behind Kernels

What does it *mean* to be a kernel?

- $K(\mathbf{x}_i, \mathbf{x}_j) = \langle \Phi(\mathbf{x}_i), \Phi(\mathbf{x}_j) \rangle$  for some  $\Phi$

What does it *take* to be a kernel?

- The Gram matrix  $G_{ij} = K(\mathbf{x}_i, \mathbf{x}_j)$ 
  - Symmetric matrix
  - Positive semi-definite matrix:  
 $\mathbf{z}^T G \mathbf{z} \geq 0$  for every non-zero vector  $\mathbf{z} \in \mathbb{R}^n$

Establishing “kernel-hood” from first principles is non-trivial

# A Few Good Kernels...

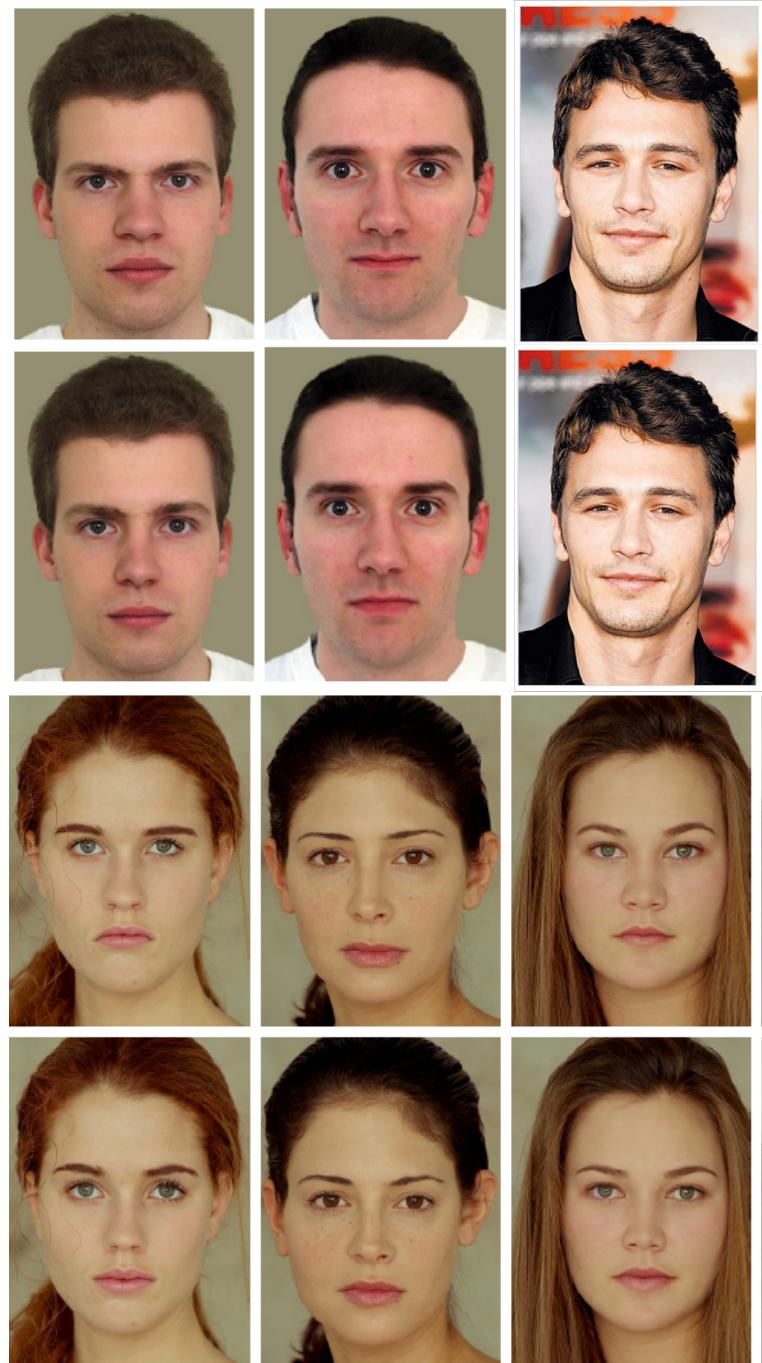
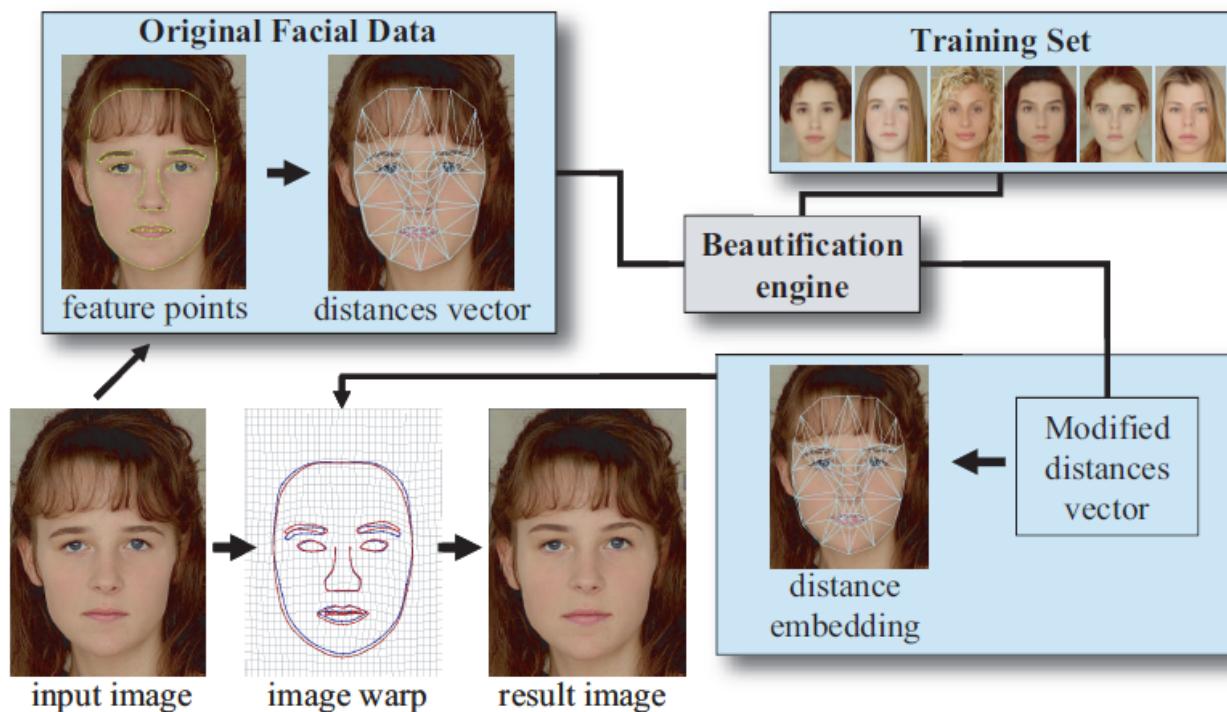
- Linear Kernel  $K(\mathbf{x}_i, \mathbf{x}_j) = \langle \mathbf{x}_i, \mathbf{x}_j \rangle$
- Polynomial kernel  $K(\mathbf{x}_i, \mathbf{x}_j) = (\langle \mathbf{x}_i, \mathbf{x}_j \rangle + c)^d$ 
  - $c \geq 0$  trades off influence of lower order terms
- Gaussian kernel  $K(\mathbf{x}_i, \mathbf{x}_j) = \exp\left(-\frac{\|\mathbf{x}_i - \mathbf{x}_j\|_2^2}{2\sigma^2}\right)$
- Sigmoid kernel  $K(\mathbf{x}_i, \mathbf{x}_j) = \tanh(\alpha \mathbf{x}_i^\top \mathbf{x}_j + c)$

Many more...

- Cosine similarity kernel
- Chi-squared kernel
- String/tree/graph/wavelet/etc kernels

# Application: Automatic Photo Retouching

(Leyvand et al., 2008)



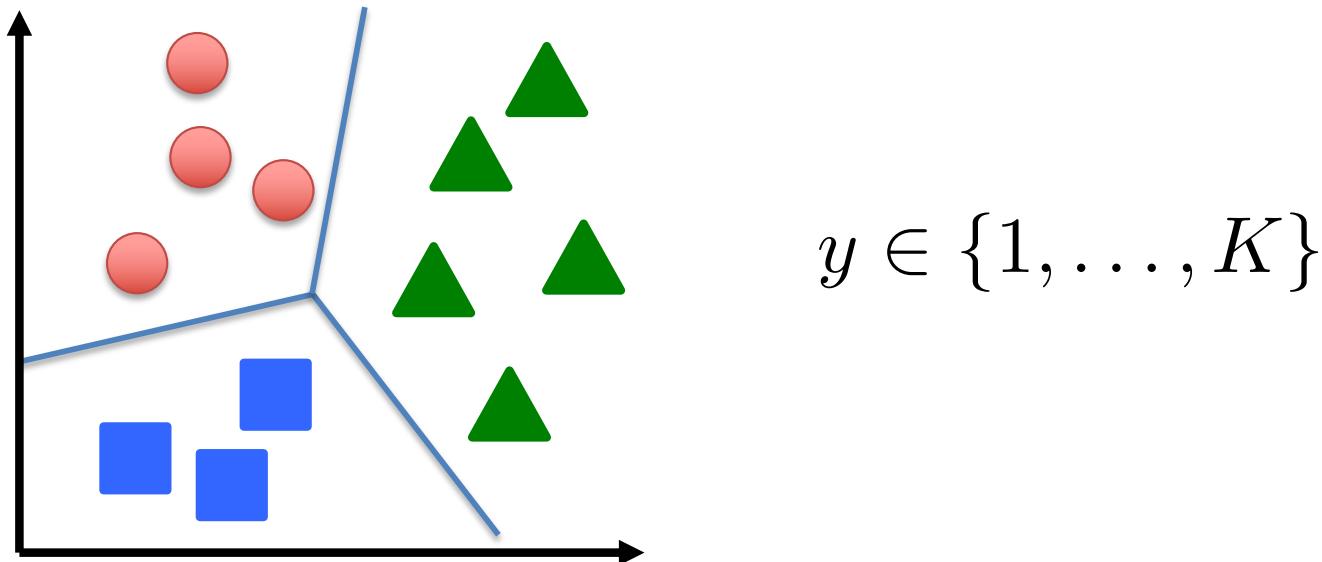
# Practical Advice for Applying SVMs

- Use SVM software package to solve for parameters
  - e.g., SVMlight, libsvm, cvx (fast!), etc.
- Need to specify:
  - Choice of parameter  $C$
  - Choice of kernel function
    - Associated kernel parameters

$$\text{e.g., } K(\mathbf{x}_i, \mathbf{x}_j) = (\langle \mathbf{x}_i, \mathbf{x}_j \rangle + c)^d$$

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

# Multi-Class Classification with SVMs



- Many SVM packages already have multi-class classification built in
- Otherwise, use one-vs-rest
  - Train  $K$  SVMs, each picks out one class from rest, yielding  $\theta^{(1)}, \dots, \theta^{(K)}$
  - Predict class  $i$  with largest  $(\theta^{(i)})^T \mathbf{x}$

# SVMs vs Logistic Regression

## (Advice from Andrew Ng)

$n$  = # training examples     $d$  = # features

If  $d$  is large (relative to  $n$ ) (e.g.,  $d > n$  with  $d = 10,000$ ,  $n = 10\text{-}1,000$ )

- Use logistic regression or SVM with a linear kernel

If  $d$  is small (up to 1,000),  $n$  is intermediate (up to 10,000)

- Use SVM with Gaussian kernel

If  $d$  is small (up to 1,000),  $n$  is large (50,000+)

- Create/add more features, then use logistic regression or SVM without a kernel

Neural networks likely to work well for most of these settings, but may be slower to train

# Other SVM Variations

- nu SVM
  - nu parameter controls:
    - Fraction of support vectors (lower bound) and misclassification rate (upper bound)
    - E.g.,  $\nu = 0.05$  guarantees that  $\geq 5\%$  of training points are SVs and training error rate is  $\leq 5\%$
  - Harder to optimize than C-SVM and not as scalable
- SVMs for regression
- One-class SVMs
- SVMs for clustering
- ...

# Conclusion

- SVMs find optimal linear separator
- The kernel trick makes SVMs learn non-linear decision surfaces
- Strength of SVMs:
  - Good theoretical and empirical performance
  - Supports many types of kernels
- Disadvantages of SVMs:
  - “Slow” to train/predict for huge data sets (but relatively fast!)
  - Need to choose the kernel (and tune its parameters)