Support Vector Machines

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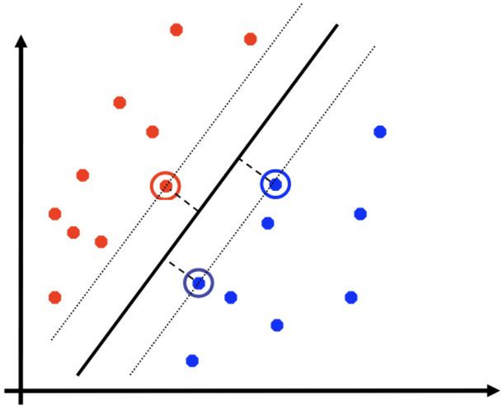
Adapted from slides by Tim Oates

Support Vector Machine

- SVMs (Vapnik, 1990's) choose the linear separator with the largest margin



V. Vapnik

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

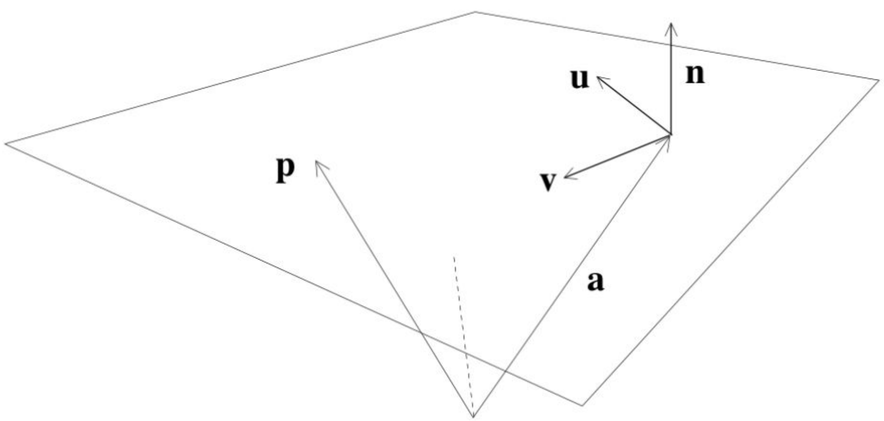
Geometry of Linear Separators

A plane can be specified as the set of all points given by:

$$\mathbf{p} = \mathbf{a} + s\mathbf{u} + t\mathbf{v}, \qquad (s,t) \in \mathcal{R}.$$

Vector from origin to a point in the plane

Two non-parallel directions in the plane



Alternatively, it can be specified as:

$$(\mathbf{p} - \mathbf{a}) \cdot \mathbf{n} = 0 \Leftrightarrow \mathbf{p} \cdot \mathbf{n} = \mathbf{a} \cdot \mathbf{n}$$

Normal vector
(we will call this w)

Only need to specify this dot product,
a scalar (we will call this the offset, b)

Notational Conventions

To better match notation used in SVMs

...and to make matrix formulas simpler

We will use the following for the i th instance

i th instance → $\mathbf{x}_i$

Bold denotes vector

i th instance label → y_i

j th feature of i th instance → x_{ij}

Non-bold denotes scalar

Linear Separators

- Training instances $\{(x_i, y_i), 1 \leq i \leq n\}$

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

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

- Model parameters

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

- Hyperplane

$$\theta^\top x = \langle \theta, x \rangle = 0$$

- Decision function

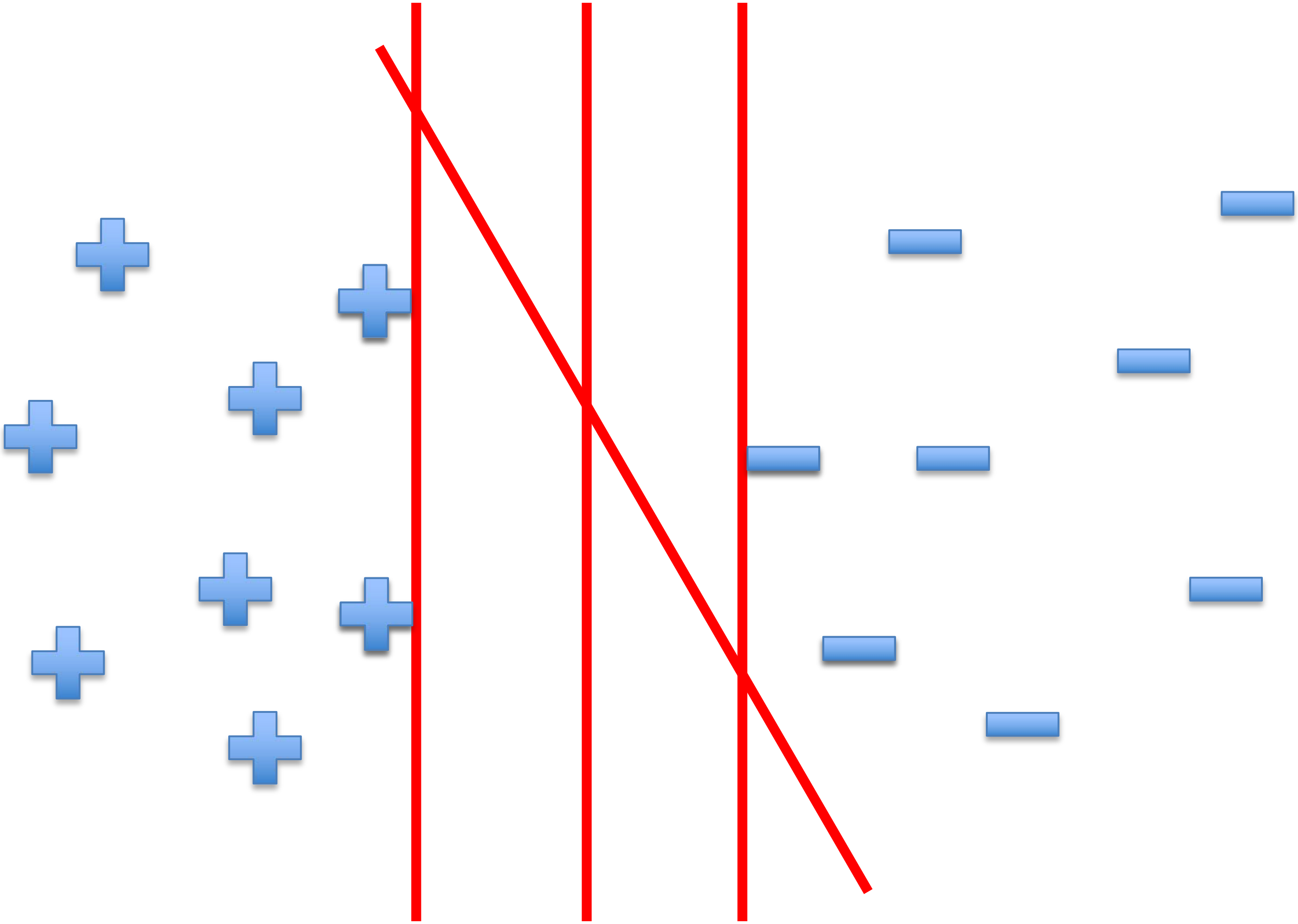
$$h(x) = sign(\theta^\top x) = sign(\langle \theta, x \rangle)$$

<u>Recall:</u>

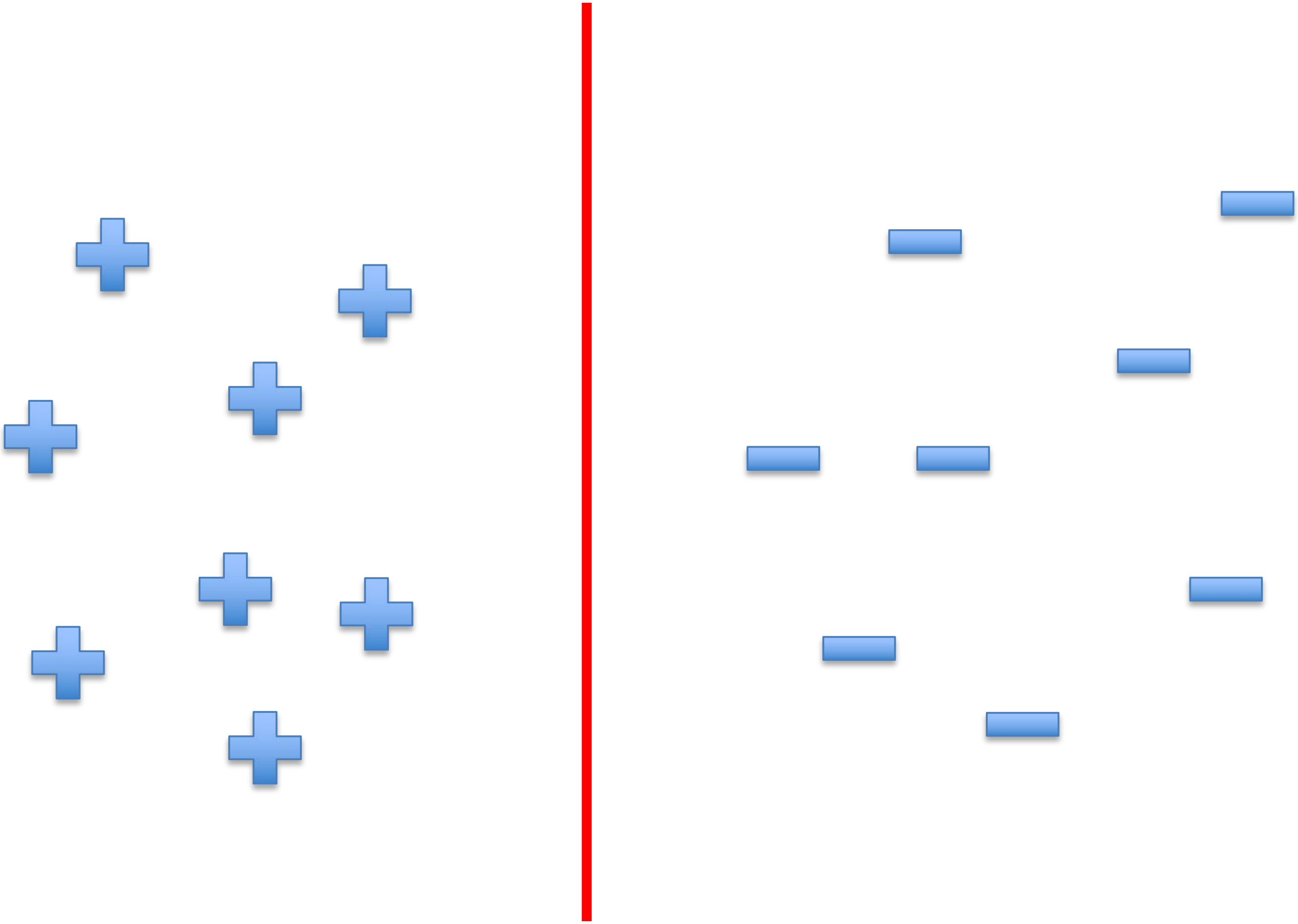
Inner (dot) product:

$$\langle \boldsymbol{u}, \boldsymbol{v} \rangle = \boldsymbol{u} \cdot \boldsymbol{v} = \boldsymbol{u}^\top v = \sum_i u_i v_i$$

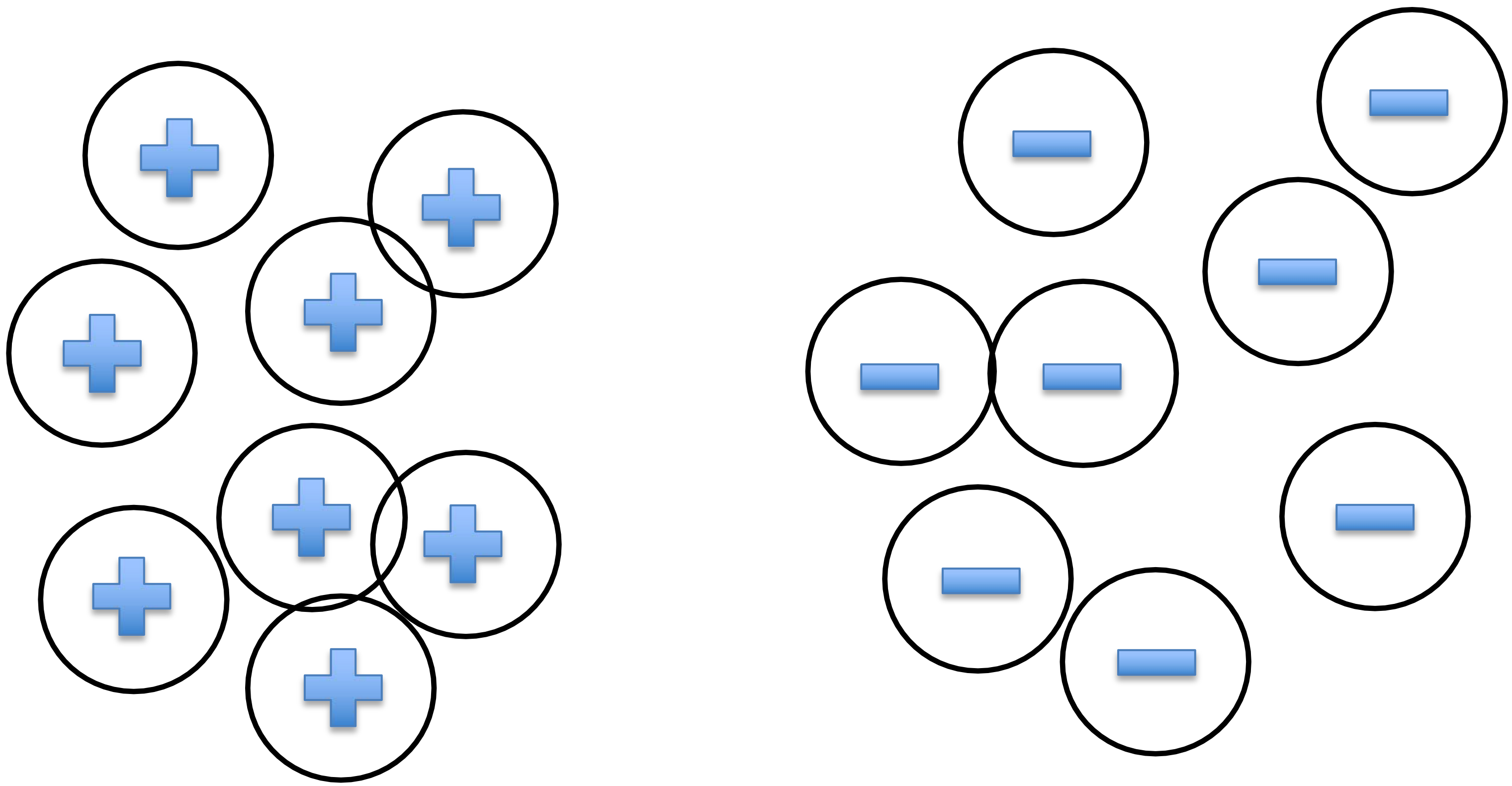
Intuitions



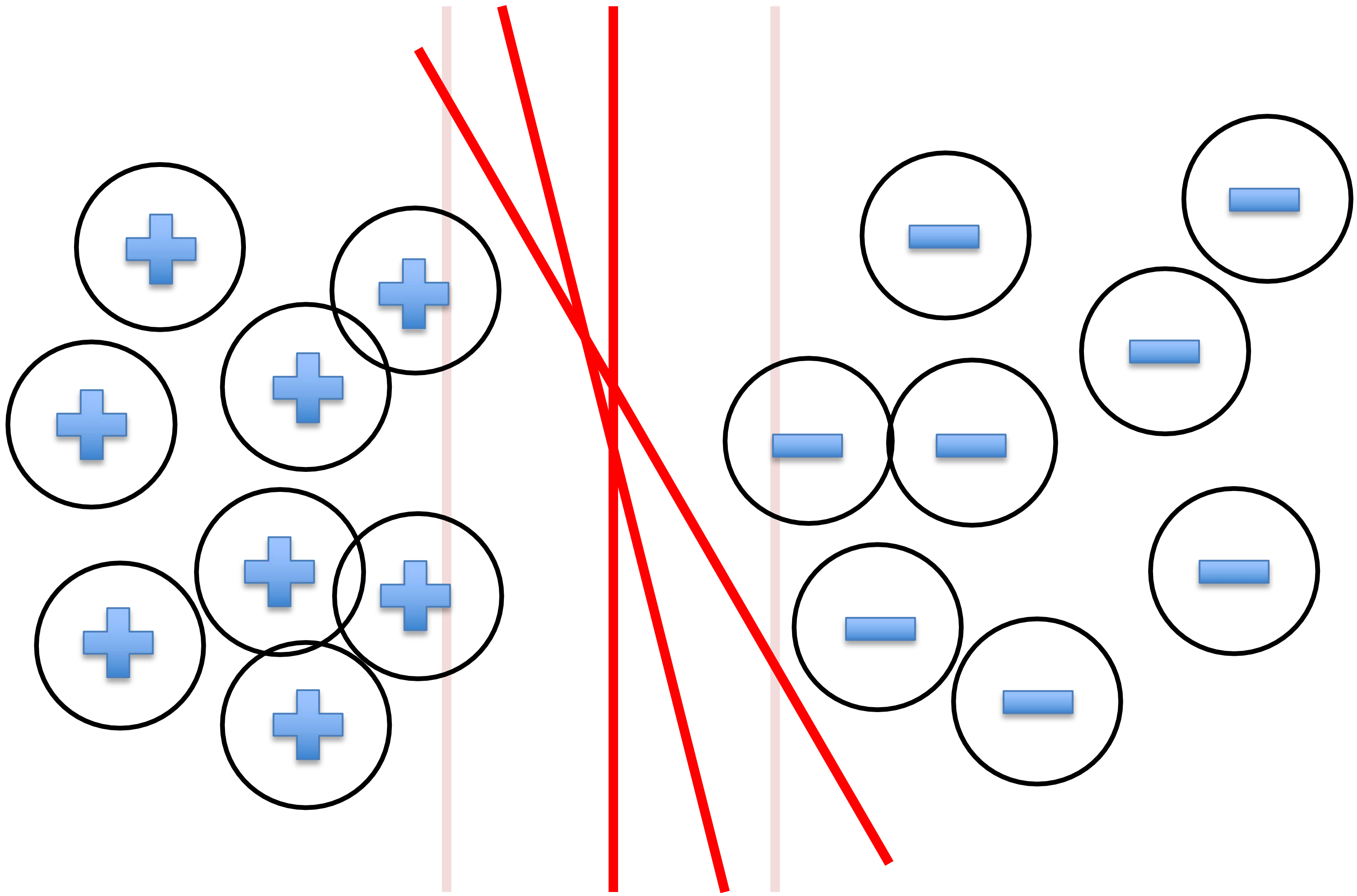
A "Good" Separator



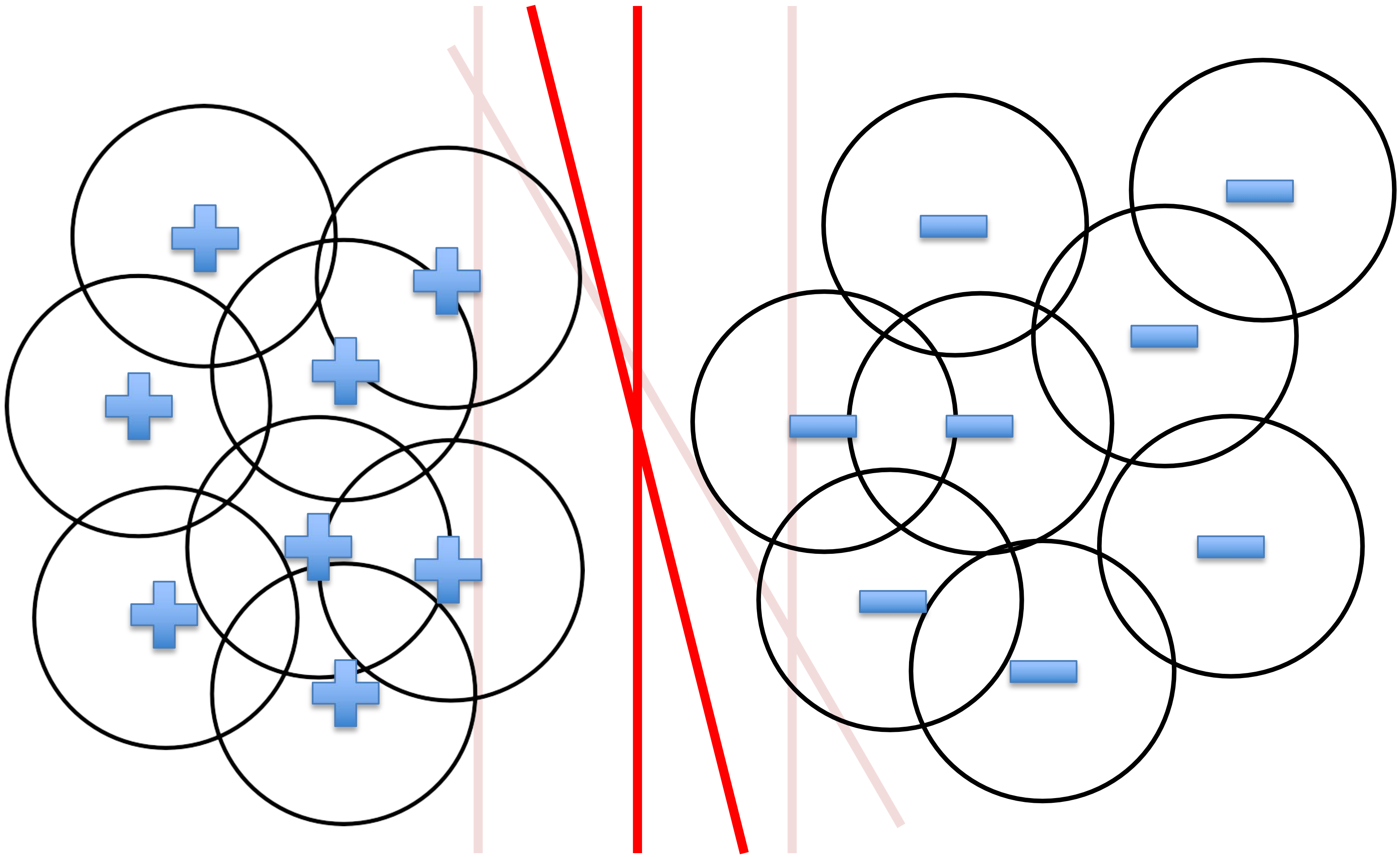
Noise in the Observations



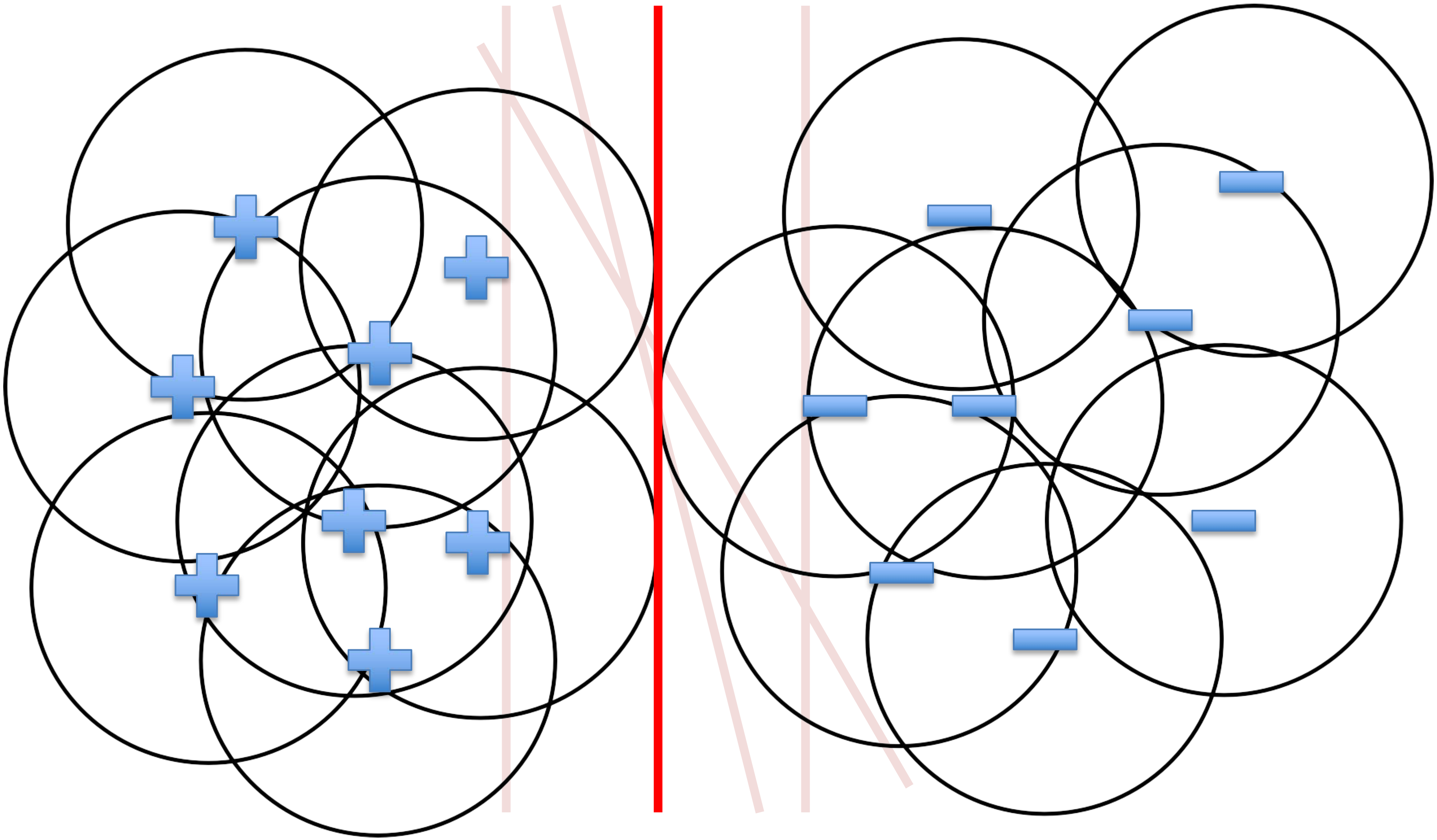
Ruling Out Some Separators



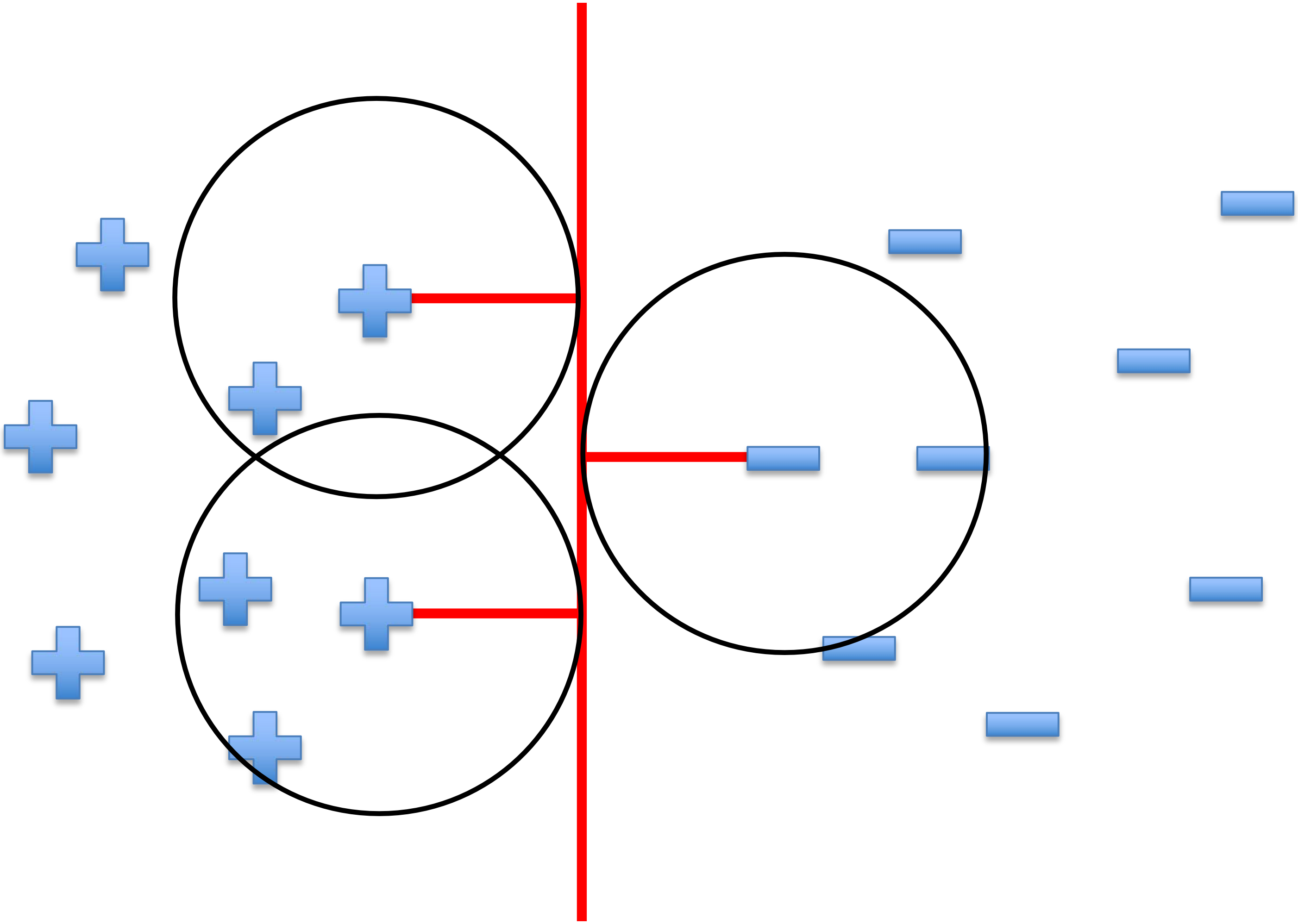
Lots of Noise



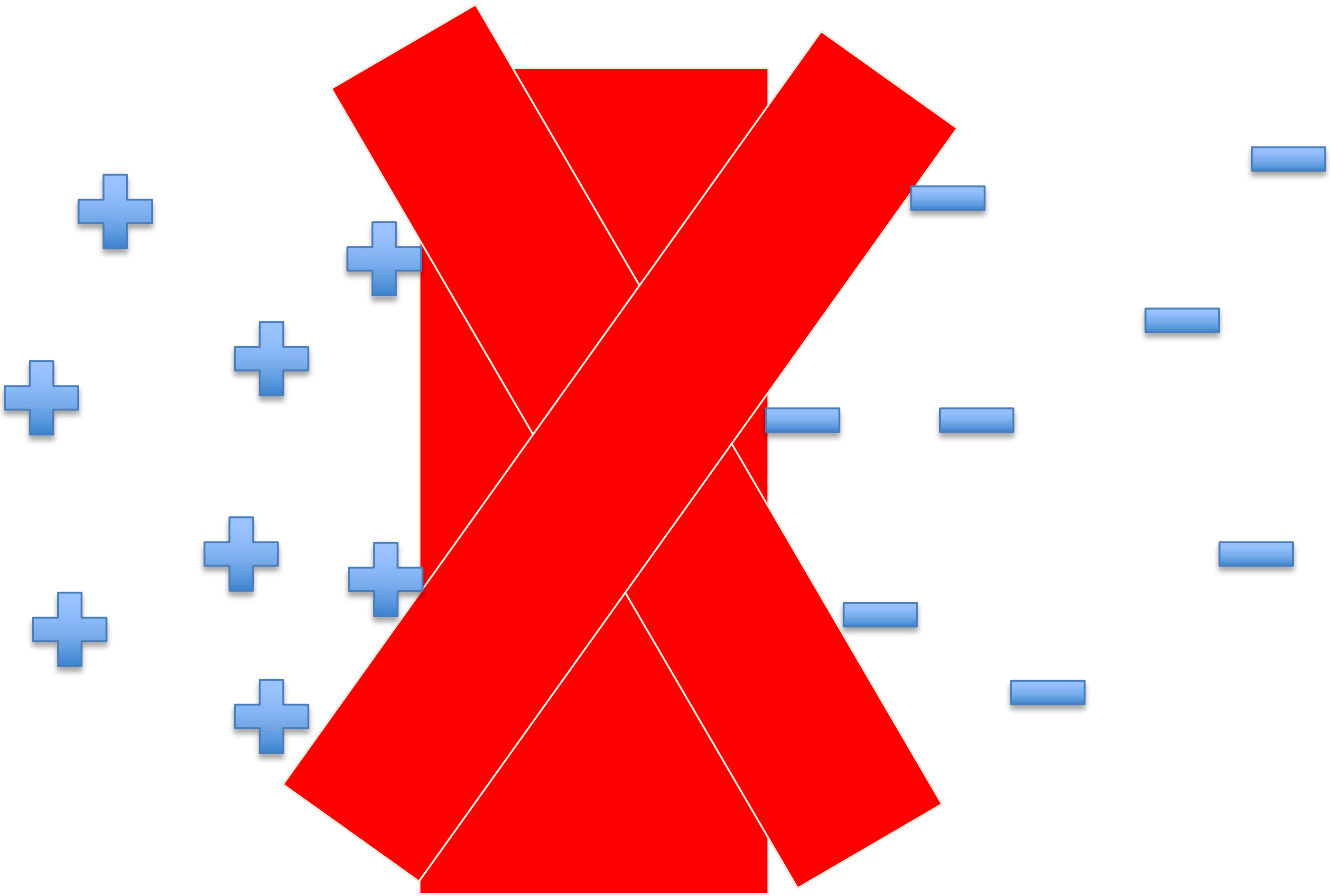
Only One Separator Remains



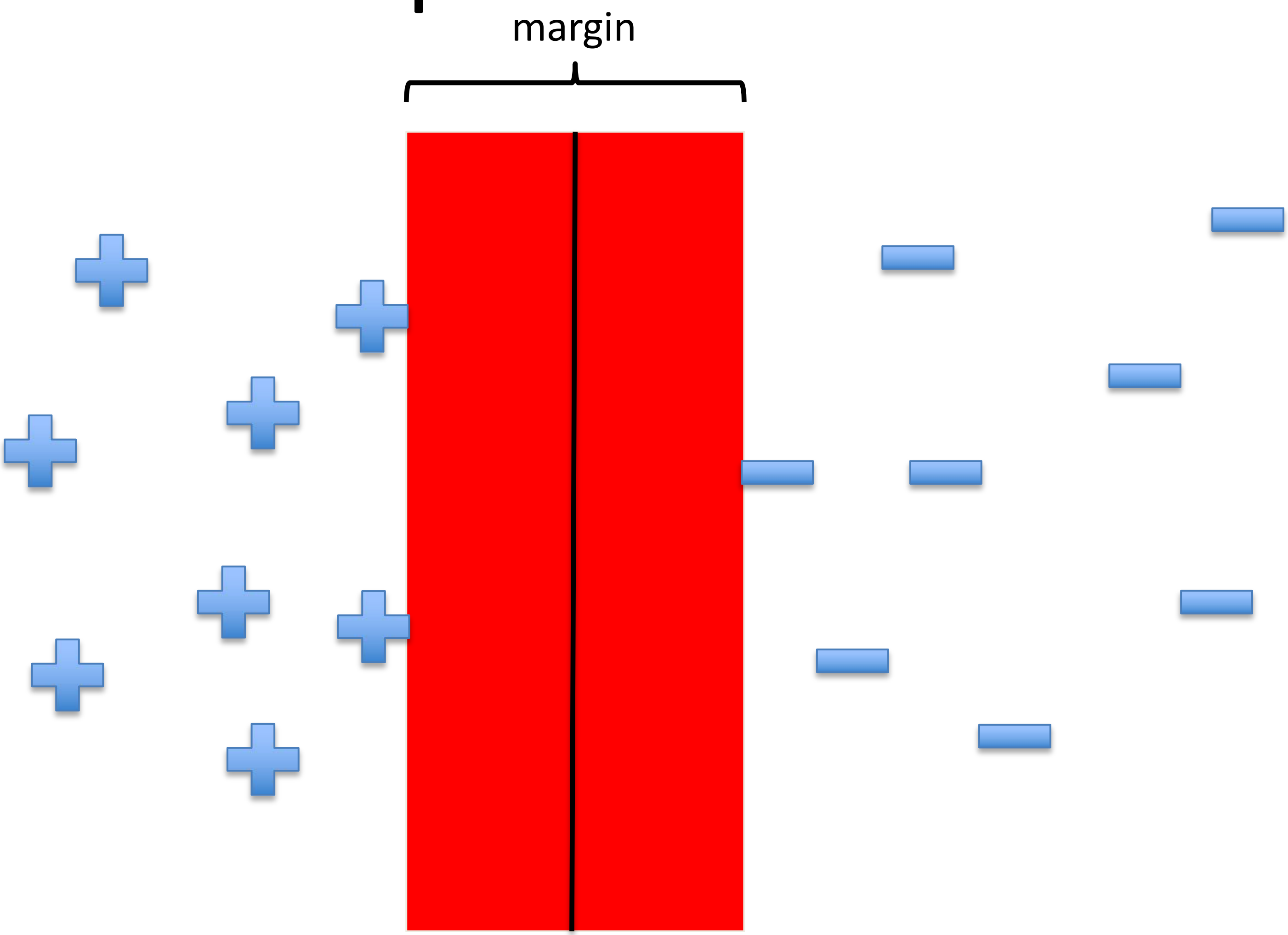
Maximizing the Margin



"Fat" Separators



"Fat" Separators



Why Maximize Margin

Increasing margin reduces *capacity*

- i.e., fewer possible models
- *What about bias? Variance?*

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

Support vector machines: 3 key ideas

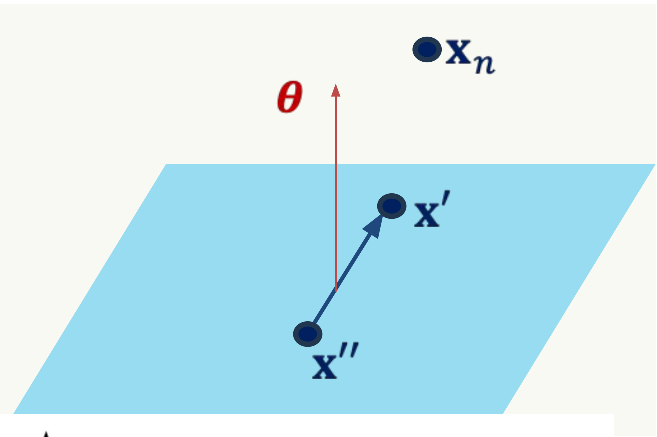
1. Use **optimization** to find solution (i.e. a hyperplane) with few errors

2. Seek **large margin** separator to improve generalization

3. Use **kernel trick** to make large feature spaces computationally efficient

Computing the margin

Margin = The distance between $\mathbf{x}_n$ and the plane $\theta^\top \mathbf{x} = 0$, such that $|\boldsymbol{\theta}^\top \mathbf{x}_n| = 1$



<u>Distance of a point to a Plane</u>

Lets say the plane is defined by $\theta^\top x = 0$

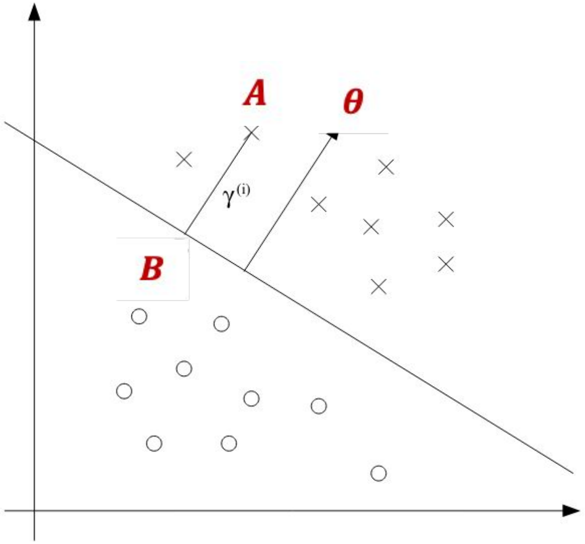
For a point A $(x^{(i)}, y^{(i)})$,

- The distance to the plane is $AB = \gamma^{(i)}$
- Point B can be obtained by $x^{(i)} - \gamma^{(i)} . \frac{\theta}{||\theta||}$
- Point B is on the plane.
- Therefore

$$\theta^\top \left(x^{(i)} - \gamma^{(i)} . \frac{\theta}{||\theta||} \right) = 0$$

<u>We can solve for $\gamma^{(i)}$ to find</u>

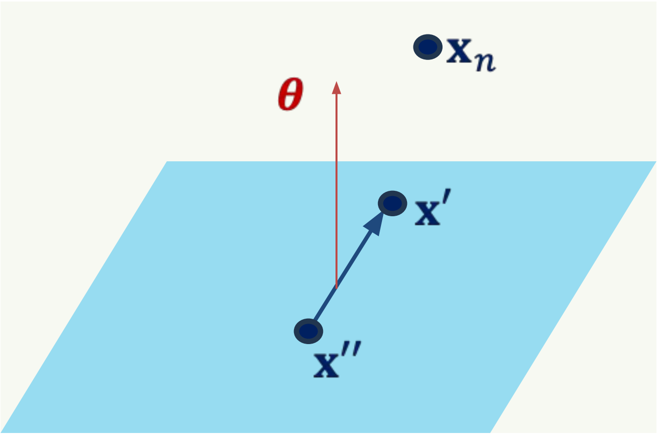
$$\gamma^{(i)} = \frac{(\theta^\top x^{(i)})}{||\theta||}$$



Computing the margin

Proposition:
The vector $\boldsymbol{\theta}$ is orthogonal to the plane in the X space

Take any two points $\mathbf{x}'$ and $\mathbf{x}''$ on the plane.



$\theta^\top \mathbf{x}' = 0$ and $\theta^\top \mathbf{x}'' = 0$
=> $\theta^\top(\mathbf{x}' - \mathbf{x}'') = 0$

Hence $\boldsymbol{\theta}$ is orthogonal to any vector that lies on the plane => $\boldsymbol{\theta}$ is orthogonal to the plane

Margin: distance between x_n and the plane

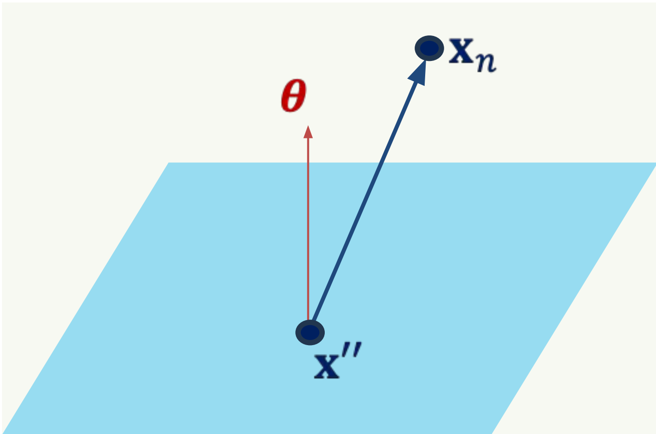
Take any point $\mathbf{x}$ on the plane

Projection of $\mathbf{x}_n - \mathbf{x}$ on $\boldsymbol{\theta}$ (direction orthogonal to the plane)

$$\widehat{\boldsymbol{\theta}} = \frac{\boldsymbol{\theta}}{||\boldsymbol{\theta}||} \Rightarrow \textbf{distance} = |\,\widehat{\boldsymbol{\theta}}^{\top}(\mathbf{x}_n - \mathbf{x})|$$

Projection of the vector $(\mathbf{x}_n - \mathbf{x})$ along $\boldsymbol{\theta}$

- computed by taking the vector product of $(\mathbf{x}_n - \mathbf{x})$ with the unit vector in the direction of $\boldsymbol{\theta}$
- $||\boldsymbol{\theta}||$ is the norm of $\boldsymbol{\theta}$

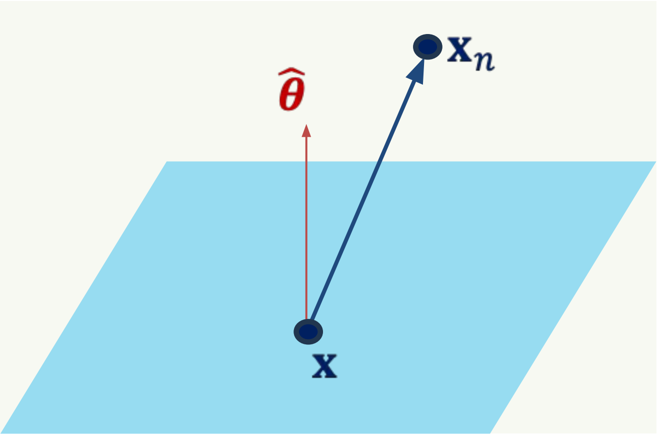


Margin: distance between x_n and the plane

$$\text{distance} = \frac{1}{||\boldsymbol{\theta}||} |\boldsymbol{\theta}^\top \mathbf{x}_n - \boldsymbol{\theta}^\top \mathbf{x}|$$

$$\frac{1}{||\boldsymbol{\theta}||} |\boldsymbol{\theta}^\top \mathbf{x}_n - \boldsymbol{\theta}^\top \mathbf{x}| = \frac{1}{||\boldsymbol{\theta}||}$$

$\mathbf{x}$ is a point on the plane.
Hence $\Rightarrow \boldsymbol{\theta}^\top \mathbf{x} = 0$
$|\boldsymbol{\theta}^\top \mathbf{x}_n| = 1$ for the nearest point $\mathbf{x}_n$ (due to our normalization)



The optimization problem

$$\text{Maximize } \frac{1}{||\boldsymbol{\theta}||}$$
$$\text{subject to } \min_{n=1,2,\ldots,N} \left| |\boldsymbol{\theta}^T \mathbf{x}_n| \right| = 1$$

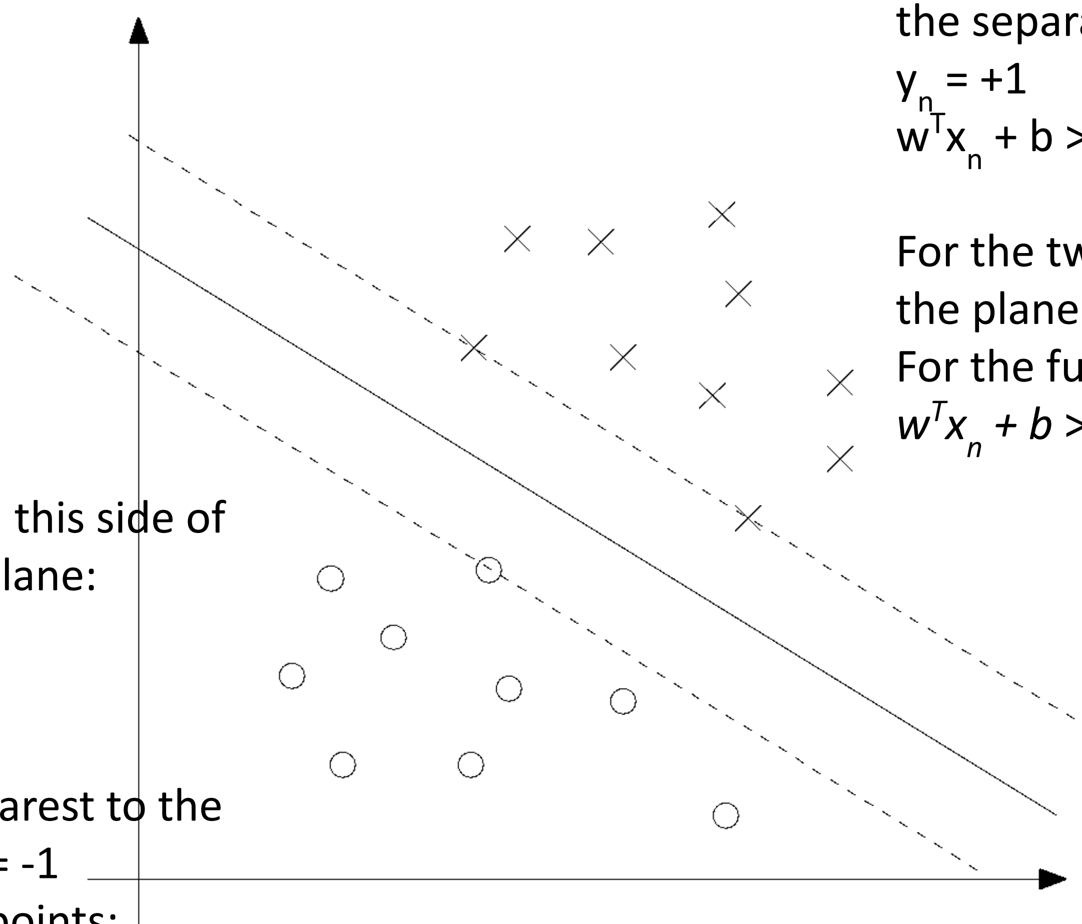
This optimization problem is too complex, because of

(i) the norm in the objective function, and

(ii) the minimum term in the constraints

Can we find an equivalent optimization problem that is easier to tackle?

The geometry



For any point on this side of the separating plane:
$y_n = +1$
$w^T x_n + b > 0$

For the two points nearest to the plane: $w^T x_n + b = 1$
For the further points:
$w^T x_n + b > 1$

For any point on this side of the separating plane:
$y_n = -1$
$w^T x_n + b < 0$

For the point nearest to the plane: $w^T x_n + b = -1$
For the further points:
$w^T x_n + b < -1$

Notice: $|\boldsymbol{\theta}^\top \mathbf{x}_n| = y_n(\boldsymbol{\theta}^\top \mathbf{x}_n)$

Equivalent optimization problem

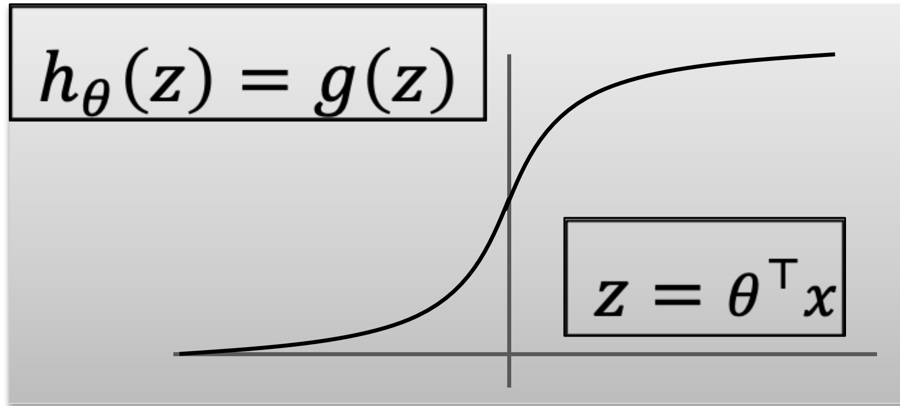
$$\text{Maximize } \frac{1}{||\boldsymbol{\theta}||}$$
$$\text{subject to } \min_{n=1,2,\ldots,N} |\boldsymbol{\theta}^\top \mathbf{x}_n| = 1$$

Notice: $|\boldsymbol{\theta}^\top \mathbf{x}_n| = y_n(\boldsymbol{\theta}^\top \mathbf{x}_n)$

$$\text{Minimize } \frac{1}{2}\boldsymbol{\theta}^\top \boldsymbol{\theta}$$
$$\text{subject to } y_n(\boldsymbol{\theta}^\top x_n) \geq 1, \text{ for } n = 1,2,\ldots N$$

Alternative View of Logistic Regression

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



If $y = 1$, we want $h_\theta(x) \approx 1$,$\theta^\top x \gg 0$

If $y = 1$, we want $h_\theta(x) \approx 0$,$\theta^\top x \ll 0$

$$J(\theta) = -\sum_{i=1}^{n} [y_i \underbrace{\log h_\theta(x_i)}_{cost_1(\theta^\top x_i)} + (1 - y_i) \underbrace{\log(1 - h_\theta(x_i))}_{cost_0(\theta^\top x_i)}]$$

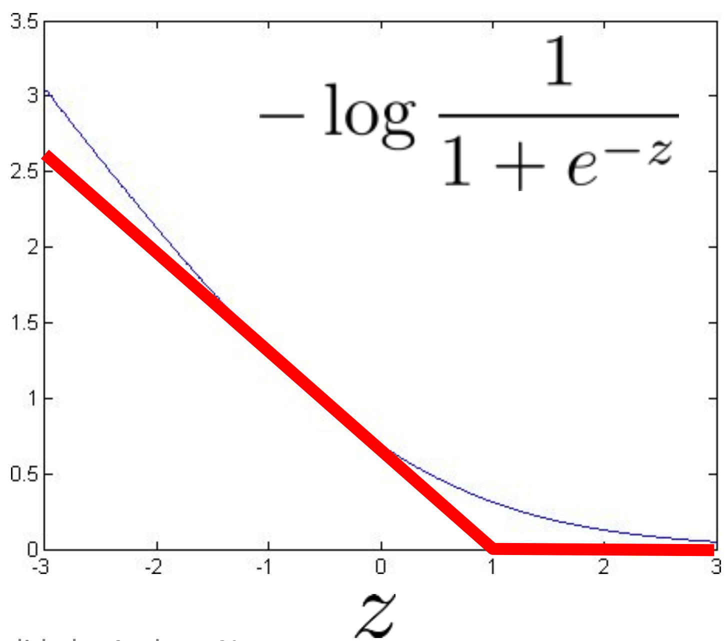
$$\min_\theta J(\theta)$$

Alternative View of Logistic Regression

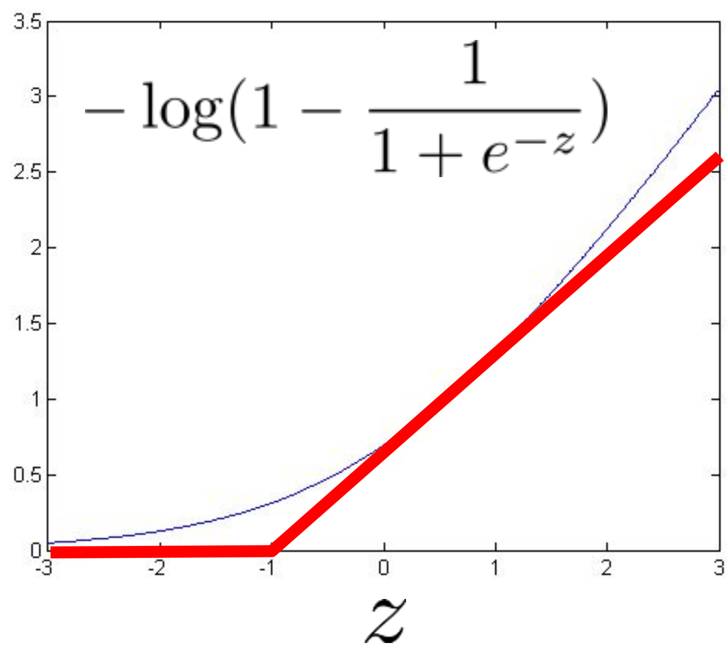
Cost of example: $-y_i \log h_{\boldsymbol{\theta}}(\mathbf{x}_i) - (1 - y_i) \log (1 - h_{\boldsymbol{\theta}}(\mathbf{x}_i))$

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

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

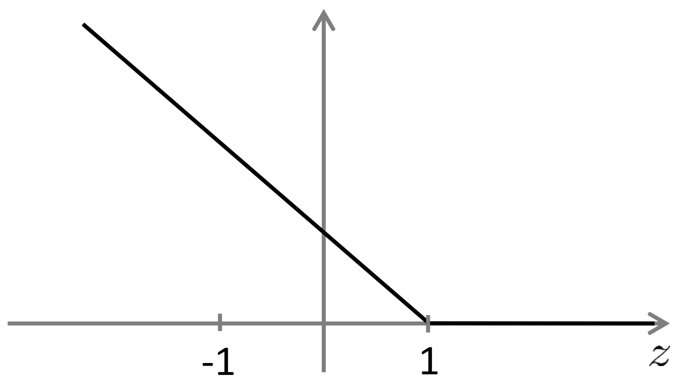


If $y = 0$ (want $\boldsymbol{\theta}^\mathsf{T}\mathbf{x} \ll 0$):

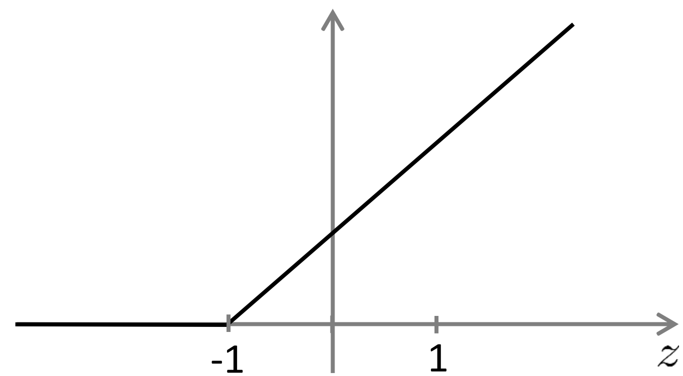


Support Vector Machine

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



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



$$l_{hinge}(h(\boldsymbol{x})) = \max(0, 1 - y \cdot h(\boldsymbol{x}))$$

Support Vector Machine

$$\min_{\theta} C \sum_{i=1}^{n} [y_i cost_1(\theta^\top x_i) + (1 - y_i) cost_0(\theta^\top x_i)] \quad + \frac{1}{2} \sum_{j=1}^{d} \theta_j^2$$

y = 1 / 0

y = +1 / -1

with C = 1

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

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

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

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