Support Vector Machines and Kernels

Doing ***Really*** Well with
Linear Decision Surfaces

Adapted from slides by Tim Oates
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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

Supervised ML = Prediction

- Given training instances (x,y)
- Learn a model f
- Such that f(x) = y
- Use f to predict y for new x
- Many variations on this basic theme

Why might predictions be wrong?

- True Non-Determinism
  - Flip a biased coin
  - p(`heads`) = θ
  - Estimate θ
  - 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?

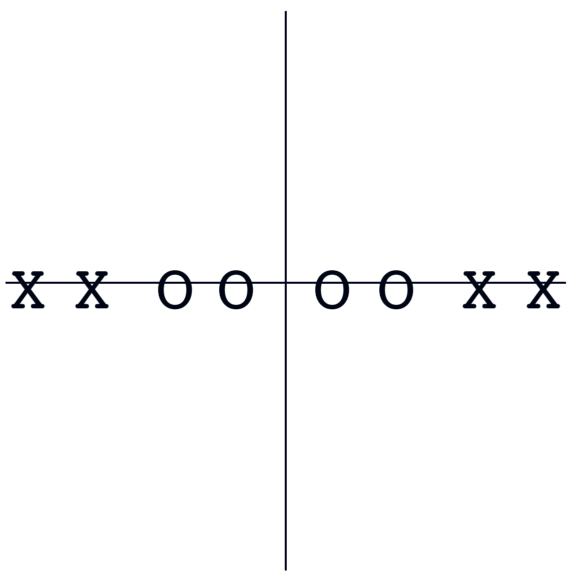
- Partial Observability
  - Something needed to predict y is missing from observation x
  - N-bit parity problem
    - x contains N-1 bits (hard PO)
    - x contains N bits but learner ignores some of them (soft PO)

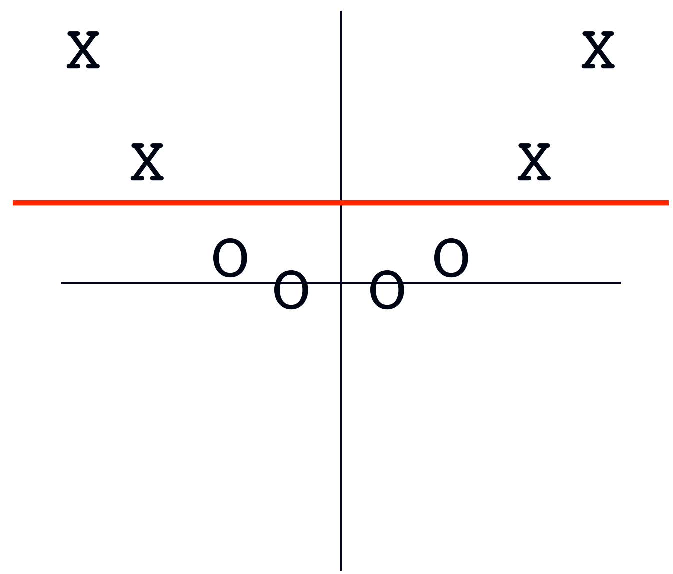
Why might predictions be wrong?

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

Linear Separators

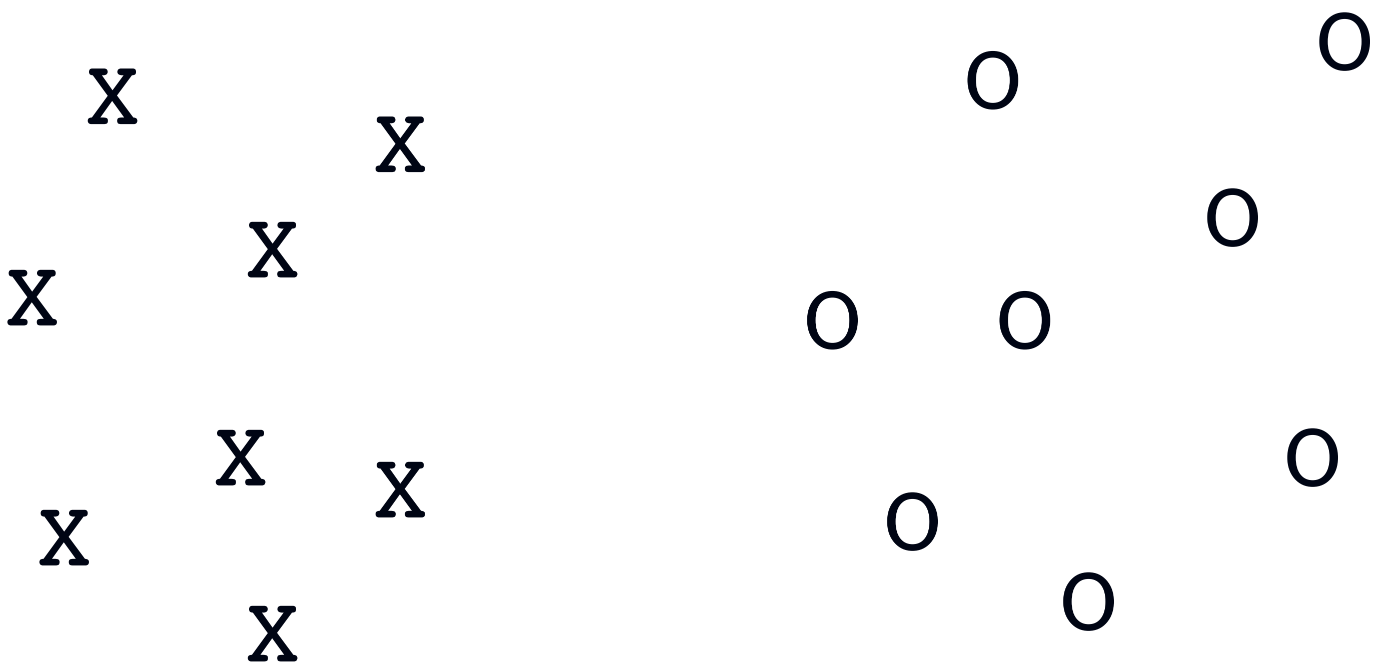
- Training instances
  - $x \in \Re^n$
  - $y \in \{-1, 1\}$
- $w \in \Re^n$
- $b \in \Re$
- Hyperplane
  - $<w, x> + b = 0$
  - $w_1 x_1 + w_2 x_2 \ldots + w_n x_n + b = 0$
- Decision function
  - $f(x) = \text{sign}(<w, x> + b)$

<u>Math Review</u>

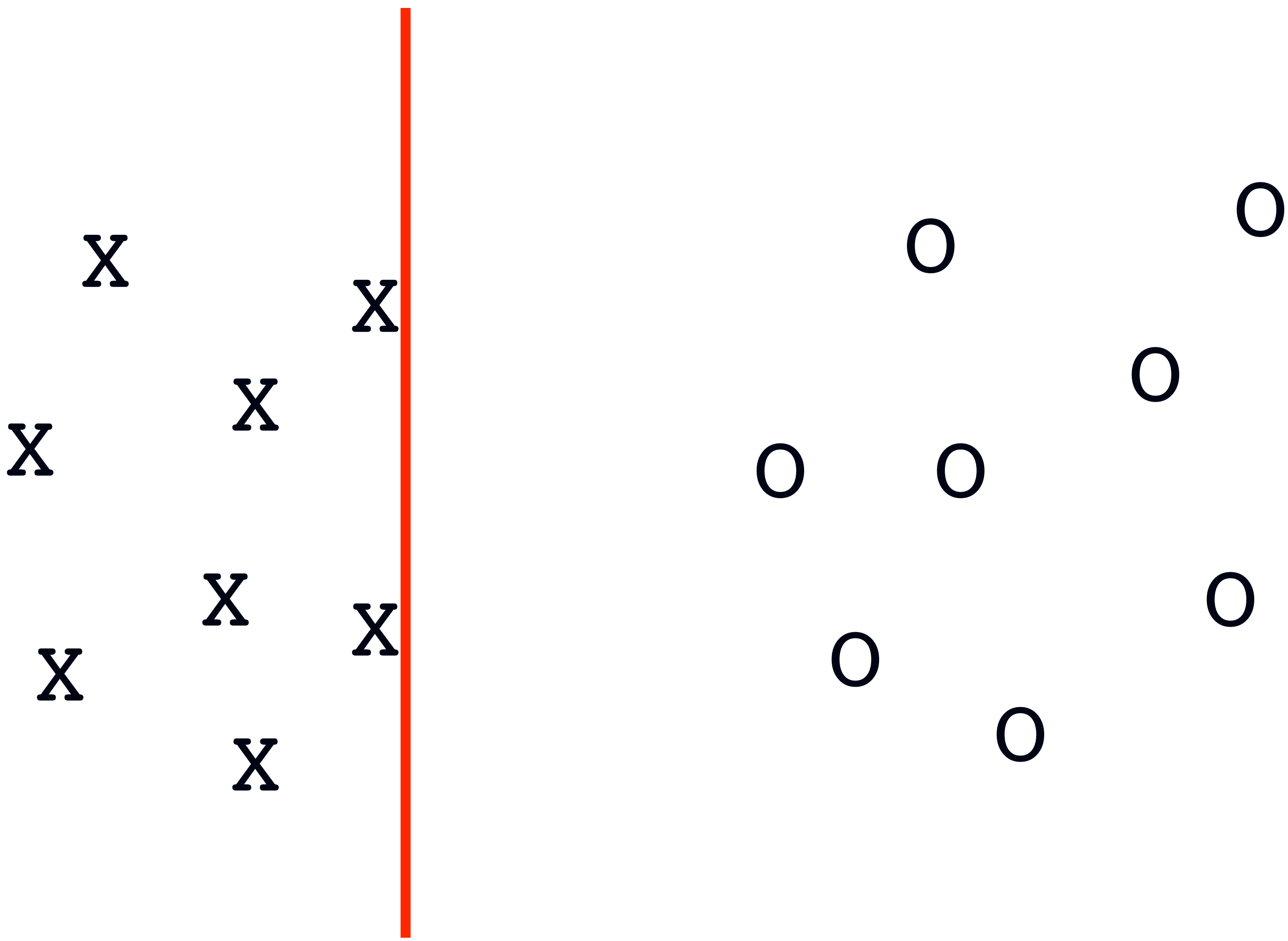
Inner (dot) product:

$$<a, b> = a \cdot b = \sum a_i {}^* b_i$$
$$= a_1 b_1 + a_2 b_2 + \ldots + a_n b_n$$

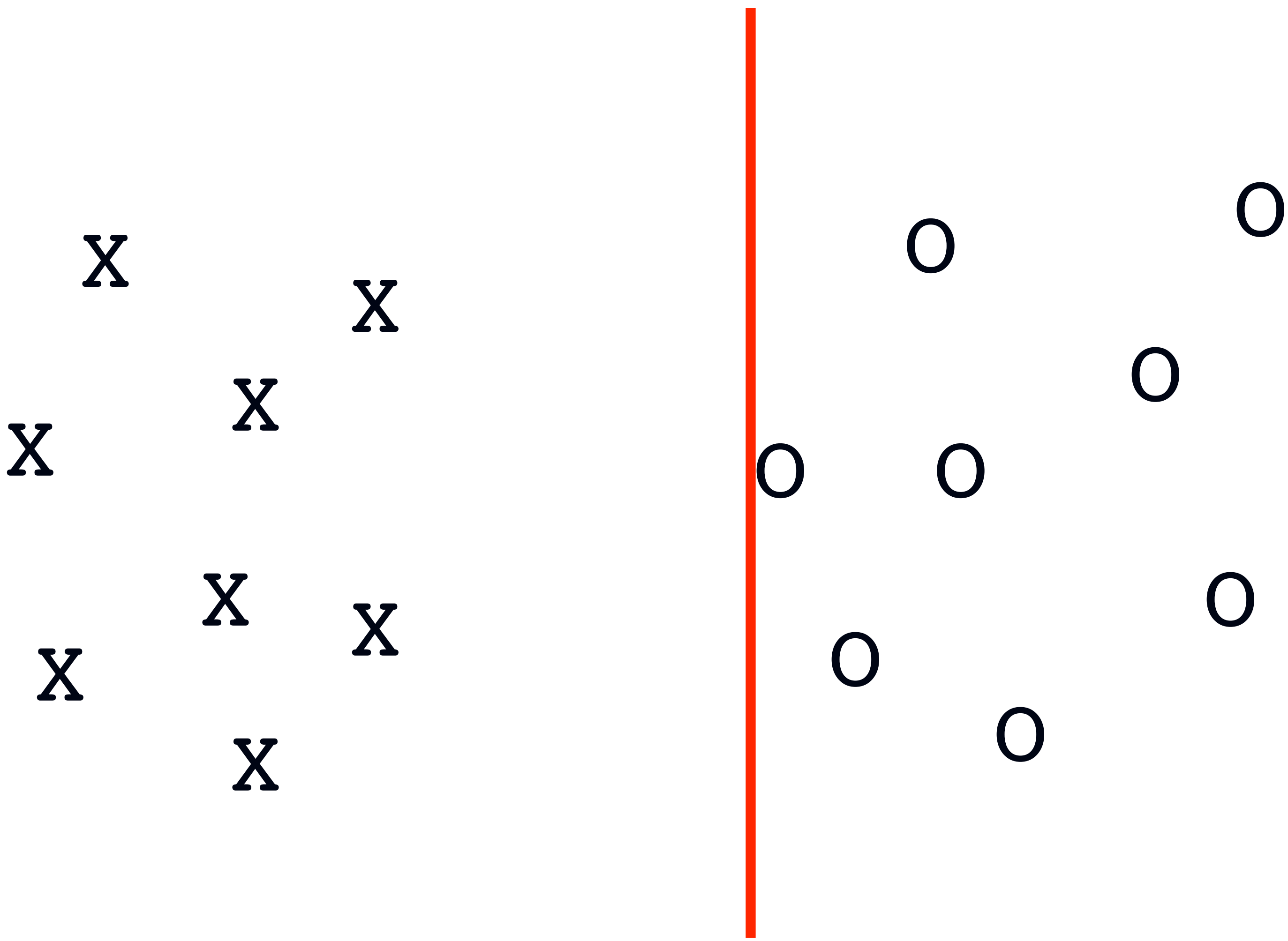
Intuitions



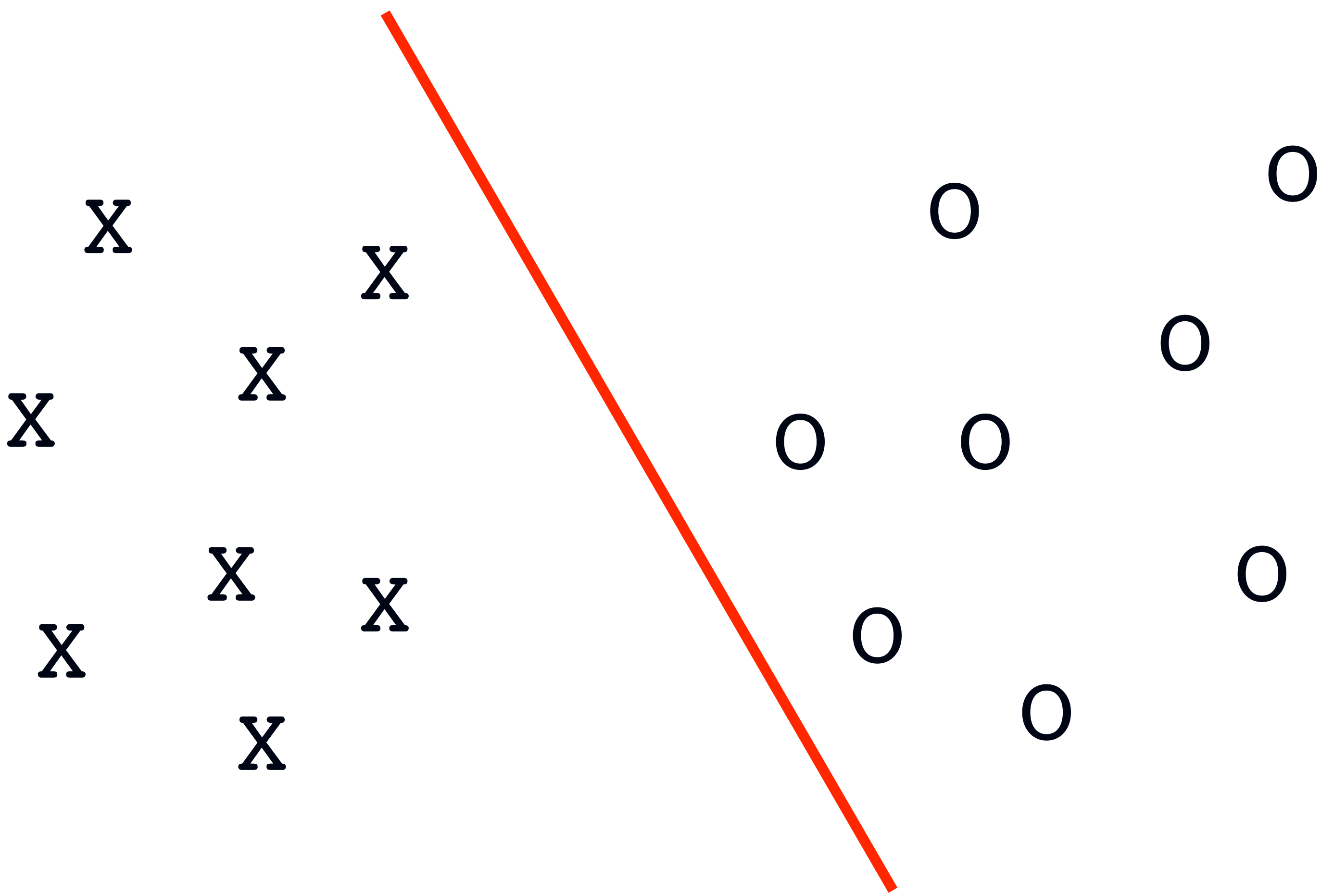
Intuitions



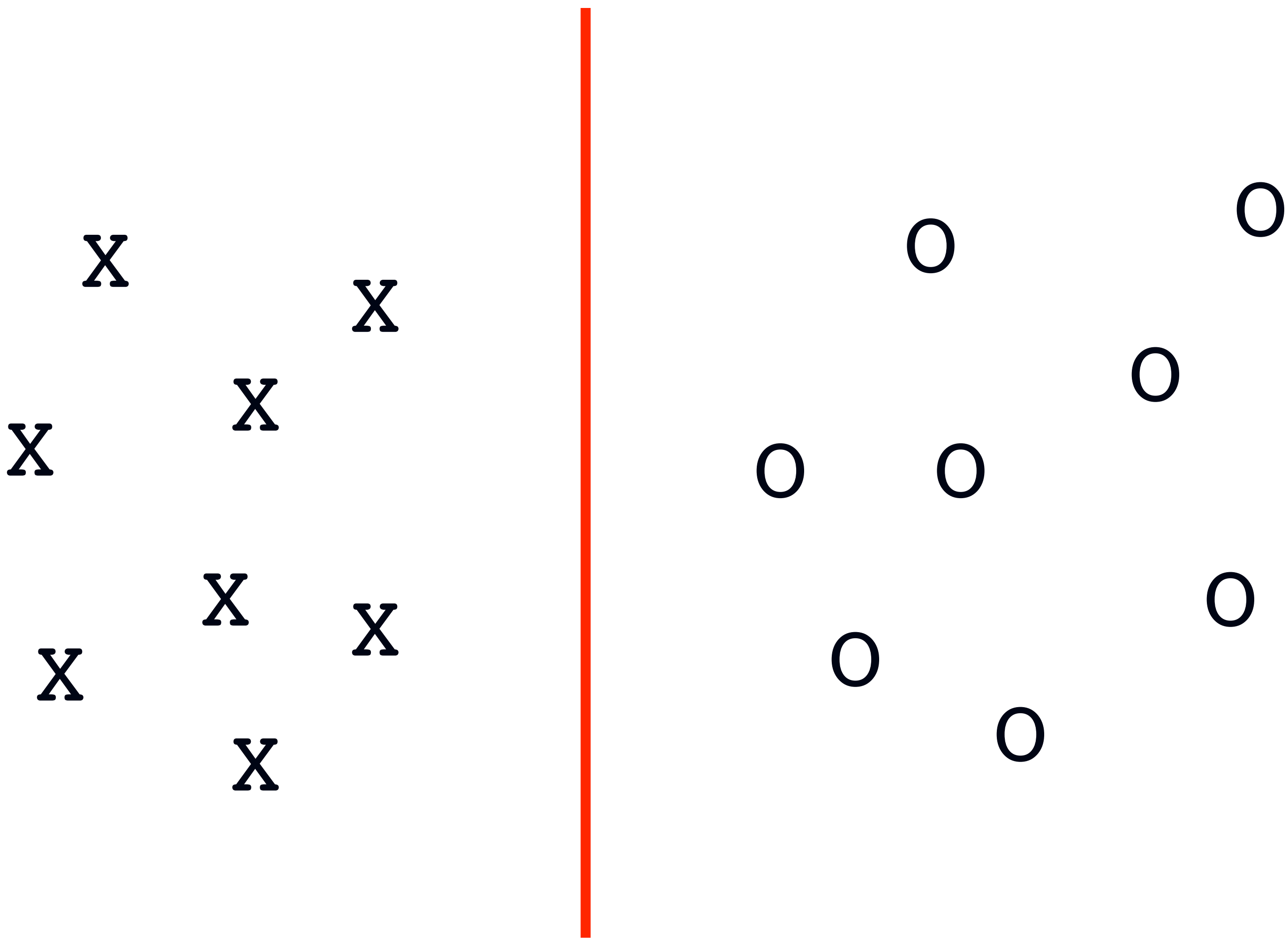
Intuitions



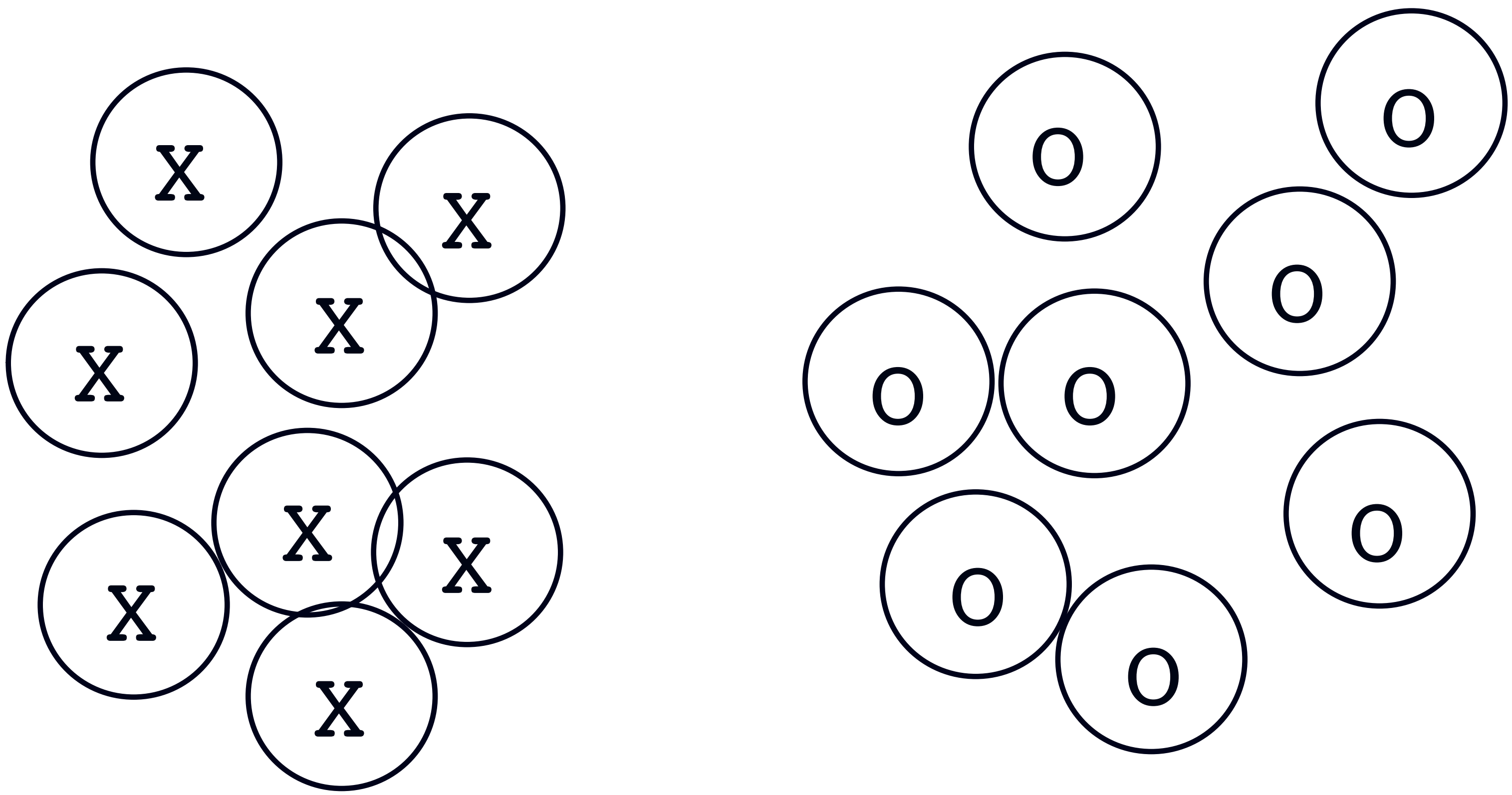
Intuitions



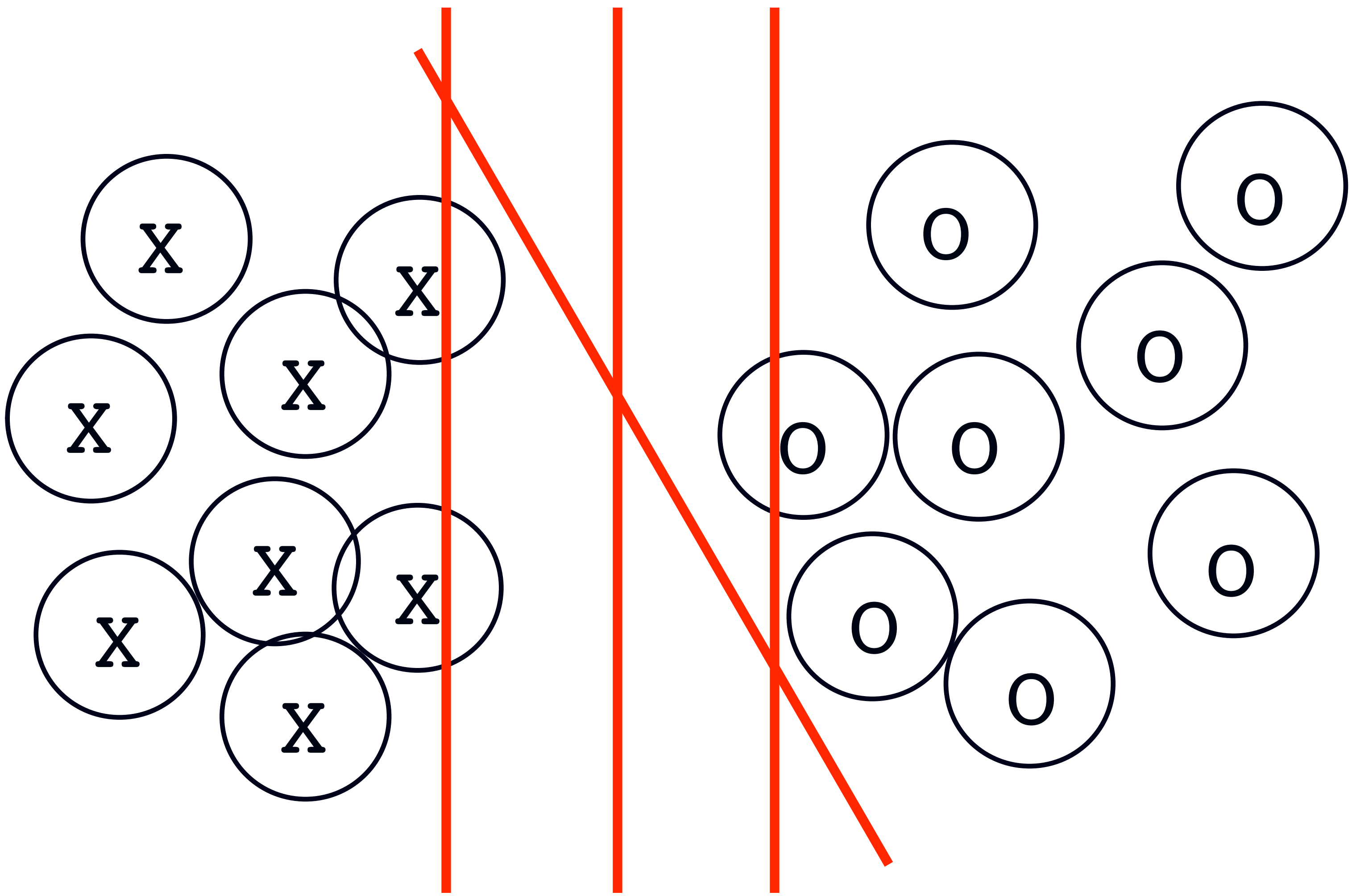
A “Good” Separator



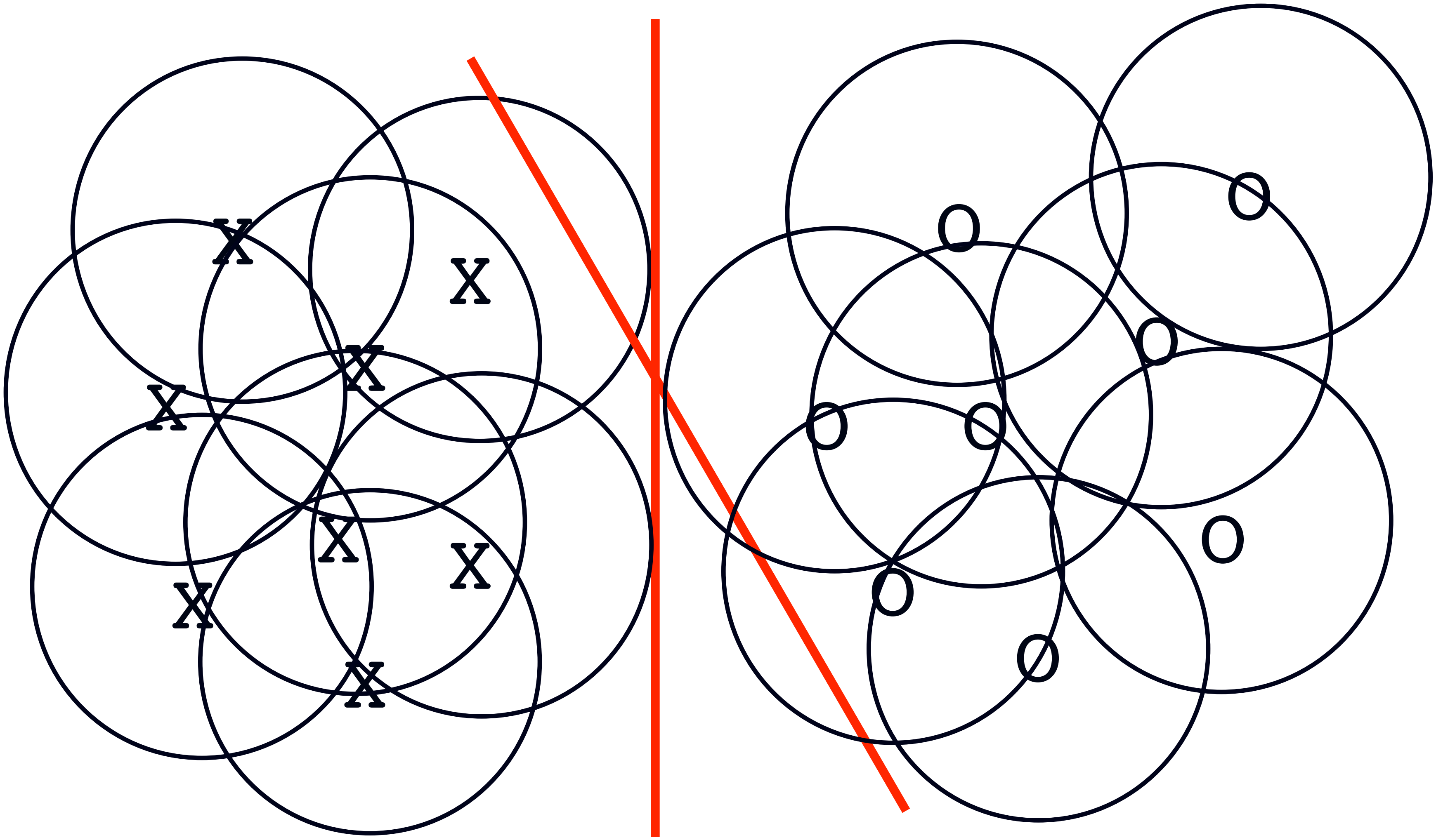
Noise in the Observations



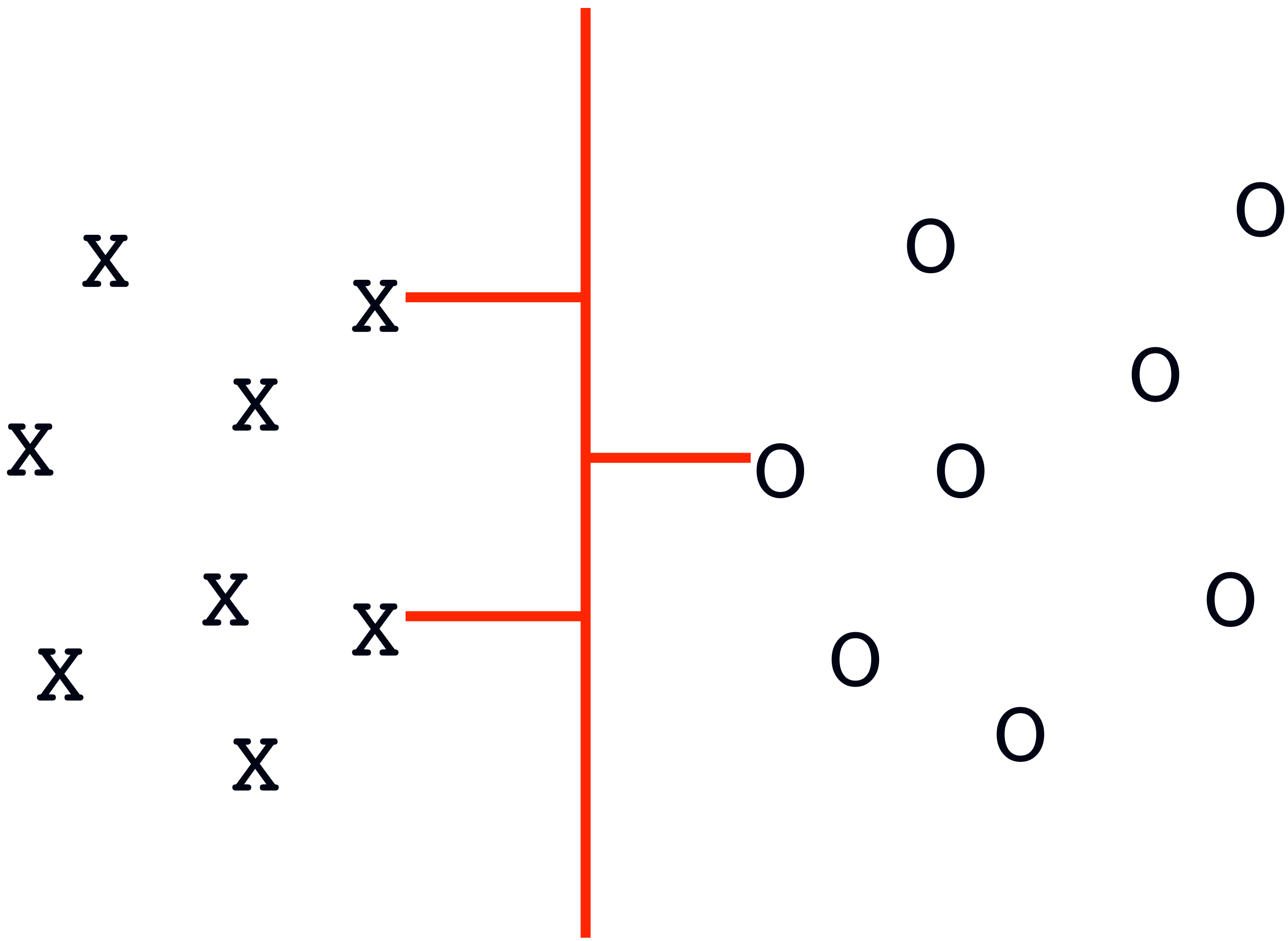
Ruling Out Some Separators



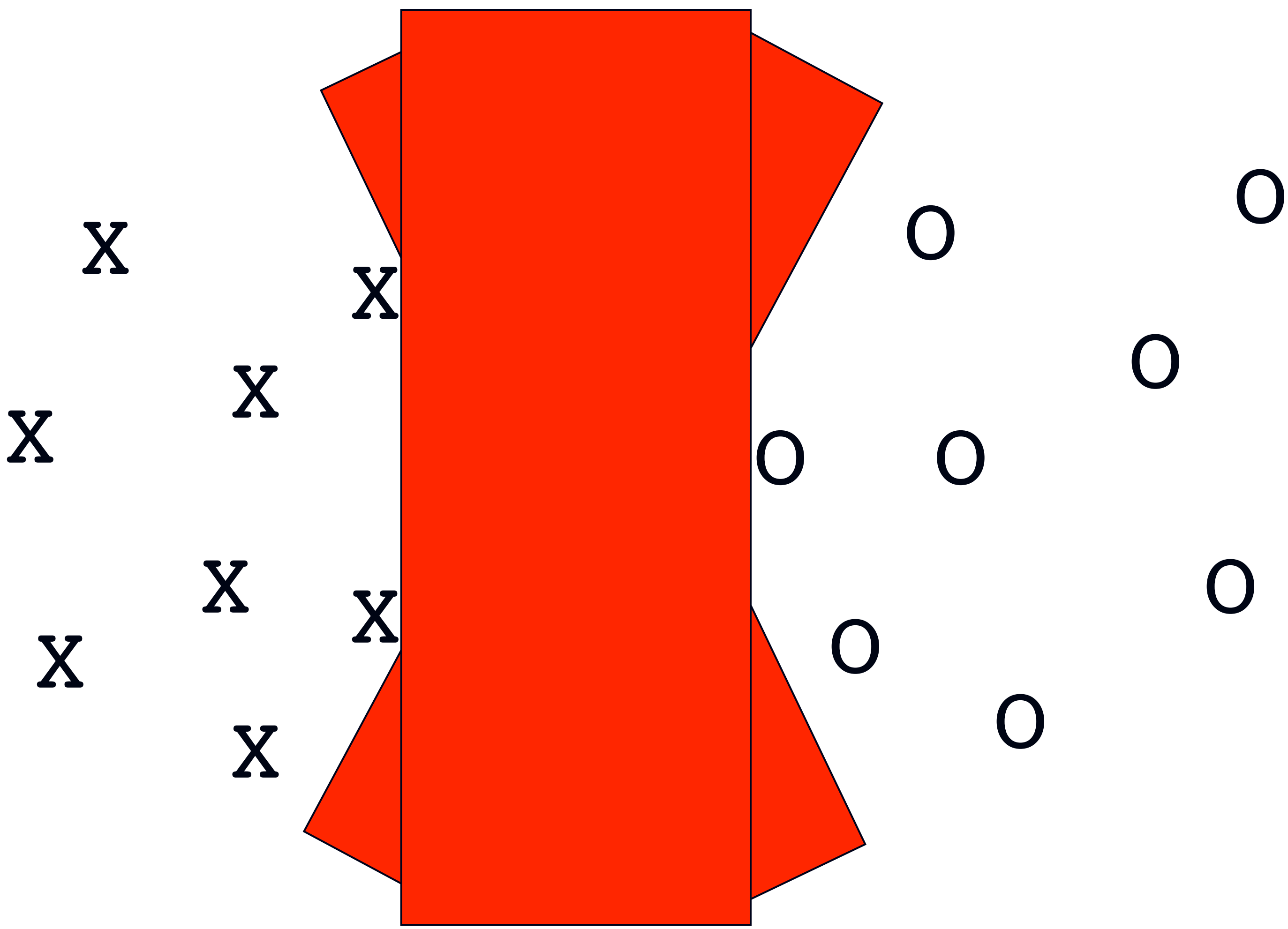
Lots of Noise



Maximizing the Margin



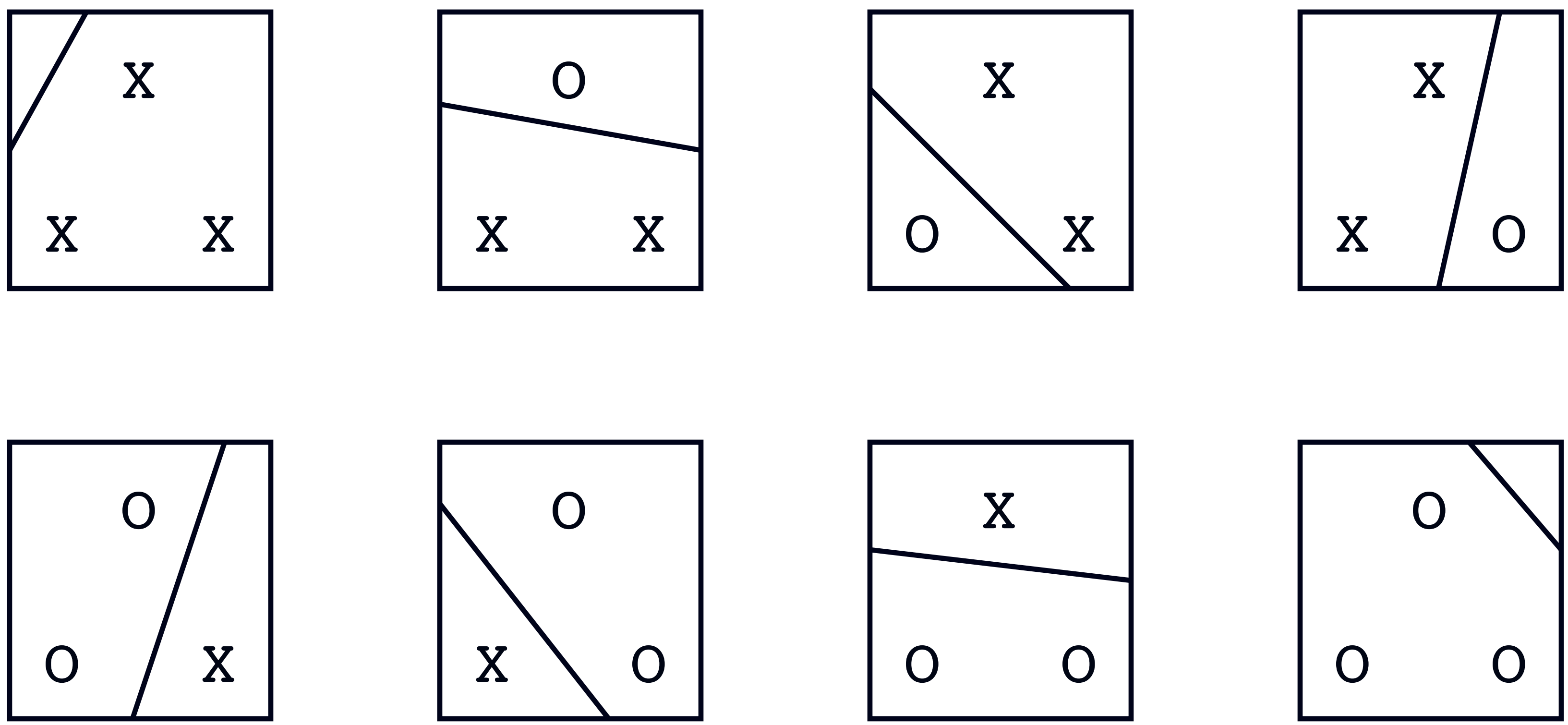
"Fat" Separators



Why Maximize Margin?

- Increasing margin reduces *capacity*
- Must restrict capacity to generalize
  - m training instances
  - 2^m ways to label them
  - What if function class that can separate them all?
  - *Shatters* the training instances
- VC Dimension is largest m such that function class can shatter some set of m points

VC Dimension Example

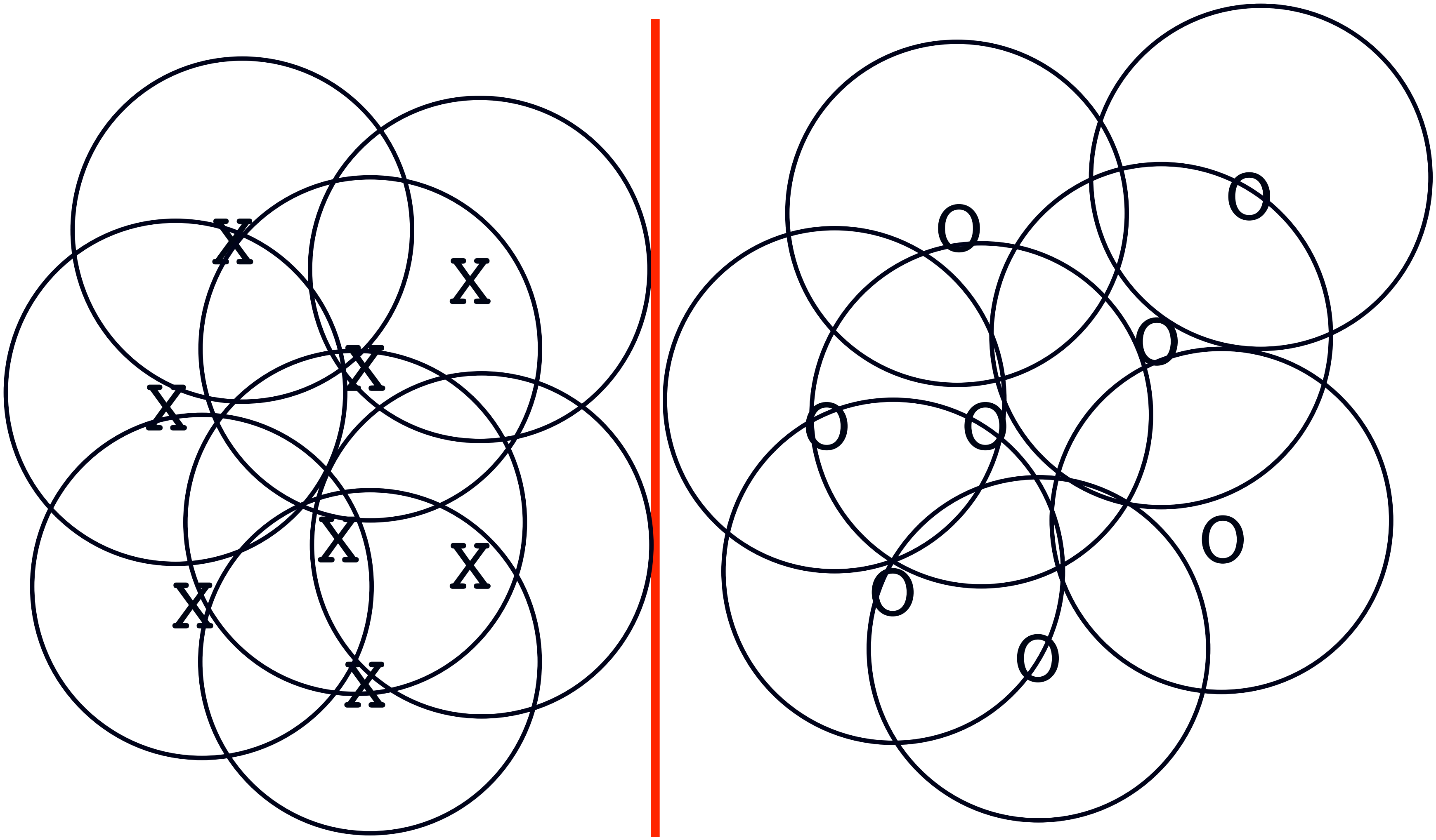


Bounding Generalization Error

- $R[f]$ = risk, test error
- $R_{emp}[f]$ = empirical risk, train error
- h = VC dimension
- m = number of training instances
- δ = probability that bound does not hold

$$R[f] \leq R_{emp}[f] + \sqrt{\frac{1}{m}\left[h\left[\ln\frac{2m}{h} + 1\right] + \ln\frac{4}{\delta}\right]}$$

Support Vectors



The Math

- Training instances
  - $x \in \Re^n$
  - $y \in \{-1, 1\}$
- Decision function
  - $f(x) = \text{sign}(\langle w,x \rangle + b)$
  - $w \in \Re^n$
  - $b \in \Re$
- Find w and b that
  - Perfectly classify training instances
    - Assuming linear separability
  - Maximize margin

The Math

- For perfect classification, we want
  - $y_i (\langle w, x_i \rangle + b) \geq 0$ for all i
  - Why?
- To maximize the margin, we want
  - w that minimizes $|w|^2$

Dual Optimization Problem

- Maximize over α
  - $W(\alpha) = \Sigma_i \alpha_i - 1/2 \, \Sigma_{i,j} \alpha_i \alpha_j y_i y_j \langle x_i, x_j \rangle$
- Subject to
  - $\alpha_i \geq 0$
  - $\Sigma_i \alpha_i y_i = 0$
- Decision function
  - $f(x) = \text{sign}(\Sigma_i \alpha_i y_i \langle x, x_i \rangle + b)$

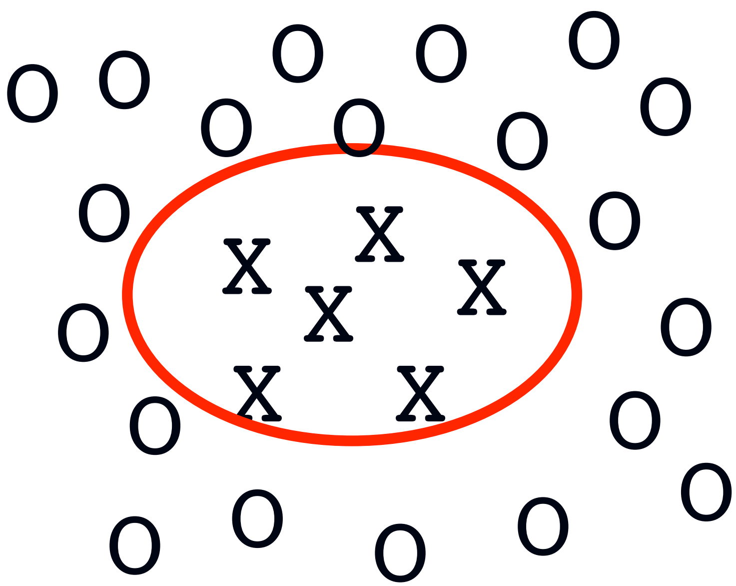
What if Data Are Not Perfectly Linearly Separable?

- Cannot find w and b that satisfy
  - $y_i (\langle w, x_i \rangle + b) \geq 1$ for all i
- Introduce slack variables ξ_i
  - $y_i (\langle w, x_i \rangle + b) \geq 1 - \xi_i$ for all i
- Minimize
  - $|w|^2 + C \Sigma \xi_i$

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?



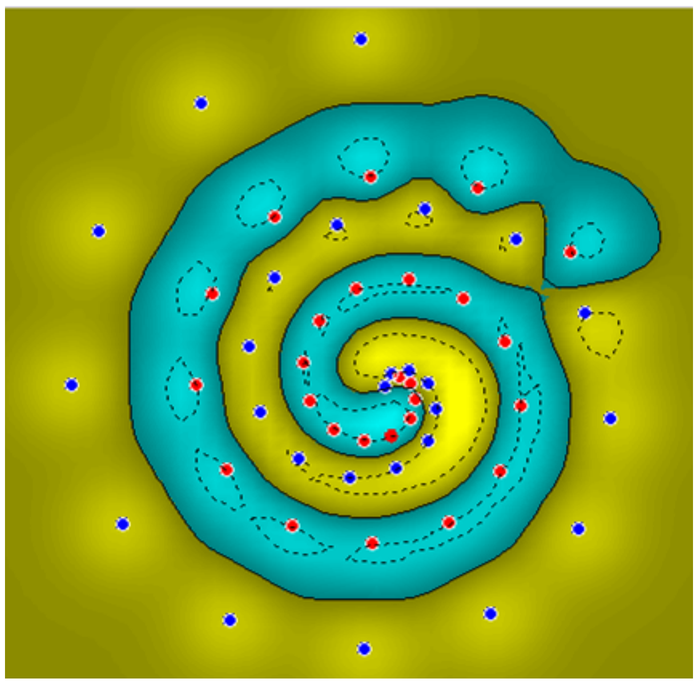
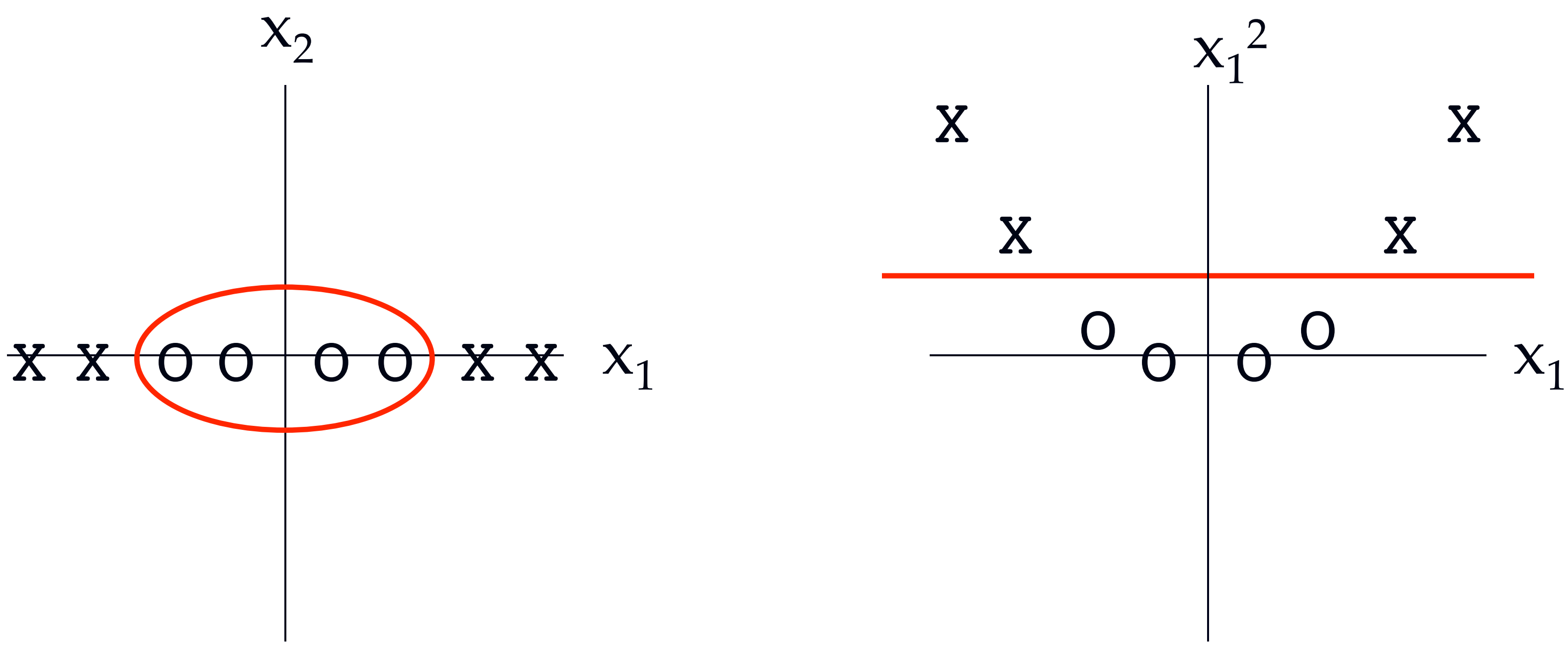


Image from http://www.atrandomresearch.com/iclass/

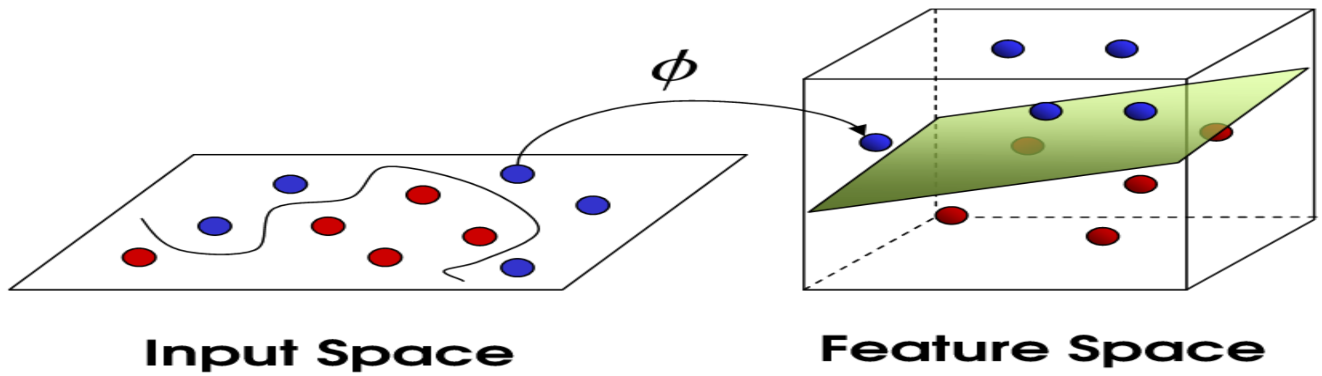
Kernel Methods

Making the Non-Linear Linear

When Linear Separators Fail



Mapping into a New Feature Space



$$\Phi : x \rightarrow X = \Phi(x)$$

$$\Phi(x_1,x_2) = (x_1,x_2,x_1^2,x_2^2,x_1x_2)$$

- Rather than run SVM on x_i, run it on $\Phi(x_i)$
- Find non-linear separator in input space
- What if $\Phi(x_i)$ is really big?
- Use kernels to compute it implicitly!

Image from http://web.engr.oregonstate.edu/~afern/classes/cs534/

Kernels

- Find kernel K such that
  - $K(x_1,x_2) = < \Phi(x_1), \Phi(x_2)>$
- Computing $K(x_1,x_2)$ should be efficient, much more so than computing $\Phi(x_1)$ and $\Phi(x_2)$
- Use $K(x_1,x_2)$ in SVM algorithm rather than $<x_1,x_2>$
- Remarkably, this is possible

The Polynomial Kernel

- $K(x_1,x_2) = \langle x_1, x_2 \rangle^2$
  - $x_1 = (x_{11}, x_{12})$
  - $x_2 = (x_{21}, x_{22})$
- $\langle x_1, x_2 \rangle = (x_{11}x_{21} + x_{12}x_{22})$
- $\langle x_1, x_2 \rangle^2 = (x_{11}^2 x_{21}^2 + x_{12}^2 x_{22}^2 + 2x_{11} x_{12} x_{21} x_{22})$
- $\Phi(x_1) = (x_{11}^2, x_{12}^2, \sqrt{2}x_{11} x_{12})$
- $\Phi(x_2) = (x_{21}^2, x_{22}^2, \sqrt{2}x_{21} x_{22})$
- $K(x_1,x_2) = \langle \Phi(x_1), \Phi(x_2) \rangle$

The Polynomial Kernel

- $\Phi(x)$ contains all monomials of degree d
- Useful in visual pattern recognition
- Number of monomials
  - 16x16 pixel image
  - 10^{10} monomials of degree 5
- Never explicitly compute $\Phi(x)$!
- Variation - $K(x_1,x_2) = (< x_1, x_2 > + 1)^2$

Kernels

- What does it *mean* to be a kernel?
  - $K(x_1,x_2) = < \Phi(x_1), \Phi(x_2) >$ for some Φ
- What does it *take* to be a kernel?
  - The Gram matrix $G_{ij} = K(x_i, x_j)$
  - Positive definite matrix
    - $\Sigma_{ij}\, c_i\, c_j\, G_{ij} \geq 0$ for $c_i, c_j \in \Re$
  - Positive definite kernel
    - For all samples of size m, induces a positive definite Gram matrix

A Few Good Kernels

- Dot product kernel
  - $K(x_1,x_2) = < x_1,x_2 >$
- Polynomial kernel
  - $K(x_1,x_2) = < x_1,x_2 >^d$ (Monomials of degree d)
  - $K(x_1,x_2) = (< x_1,x_2 > + 1)^d$ (All monomials of degree 1,2,…,d)
- Gaussian kernel
  - $K(x_1,x_2) = \exp(-| x_1-x_2 |^2/2\sigma^2)$
  - Radial basis functions
- Sigmoid kernel
  - $K(x_1,x_2) = \tanh(< x_1,x_2 > + \vartheta)$
  - Neural networks
- Establishing "kernel-hood" from first principles is non-trivial

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

Using a Different Kernel in the Dual Optimization Problem

- For example, using the polynomial kernel with d = 4 (including lower-order terms).
- Maximize over α
  - $(<x_i, x_j> + 1)^4$
  - $W(\alpha) = \Sigma_i \alpha_i - 1/2\, \Sigma_{i,j} \alpha_i \alpha_j y_i y_j \cancel{<x_i, x_j>}$
- Subject to
  - $\alpha_i \geq 0$
  - $\Sigma_i \alpha_i y_i = 0$

So by the kernel trick, we just replace them!

These are kernels!

- Decision function
  - $(<x_i, x_j> + 1)^4$
  - $f(x) = \text{sign}(\Sigma_i \alpha_i y_i \cancel{<x, x_i>} + b)$

Exotic Kernels

- Strings
- Trees
- Graphs
- The hard part is establishing kernel-hood

Conclusion

- SVMs find optimal linear separator
- The kernel trick makes SVMs non-linear learning algorithms