



Support Vector Machines & Kernels

Doing *really* well with linear decision surfaces

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Understanding the Dual

$$\begin{aligned} \text{Maximize } J(\boldsymbol{\alpha}) &= \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j y_i y_j \langle \mathbf{x}_i, \mathbf{x}_j \rangle \\ \text{s. t. } \alpha_i &\geq 0 \quad \forall i \\ \sum_i \alpha_i y_i &= 0 \end{aligned}$$

In the solution, either:

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

Understanding the Dual

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The decision function is given by

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

What if Data Are Not Linearly Separable?

Cannot find θ that satisfies. $y_i(\theta^T x_i) \geq 1 \forall i$

Introduce slack variables ξ_i

$$y_i(\theta^T x_i) \geq 1 - \xi_i \quad \forall i$$

New Problem

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

$$\text{s. t. } y_i(\theta^T x_i) \geq 1 - \xi_i, \quad \text{if } \forall i$$

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?

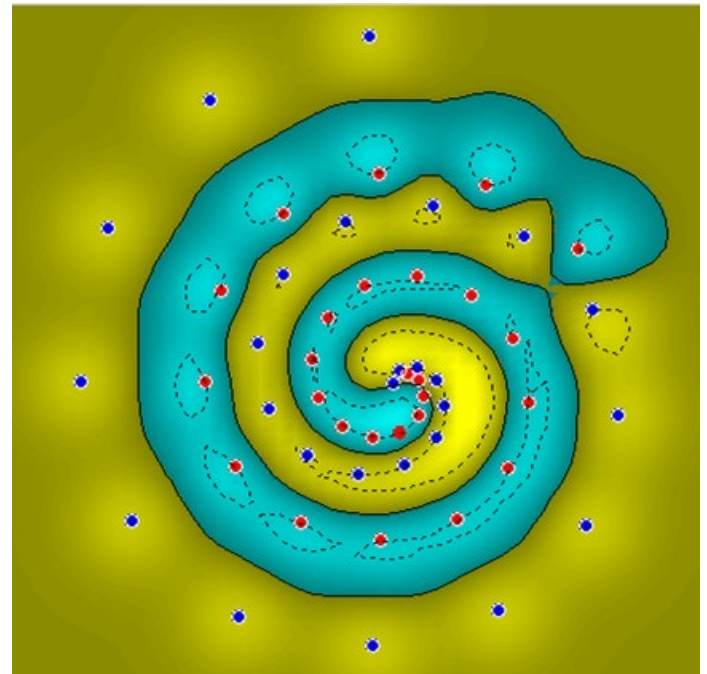
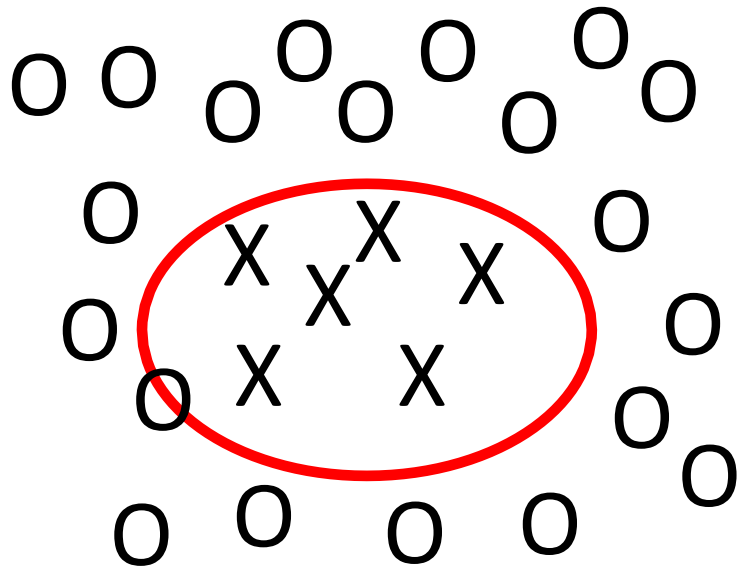
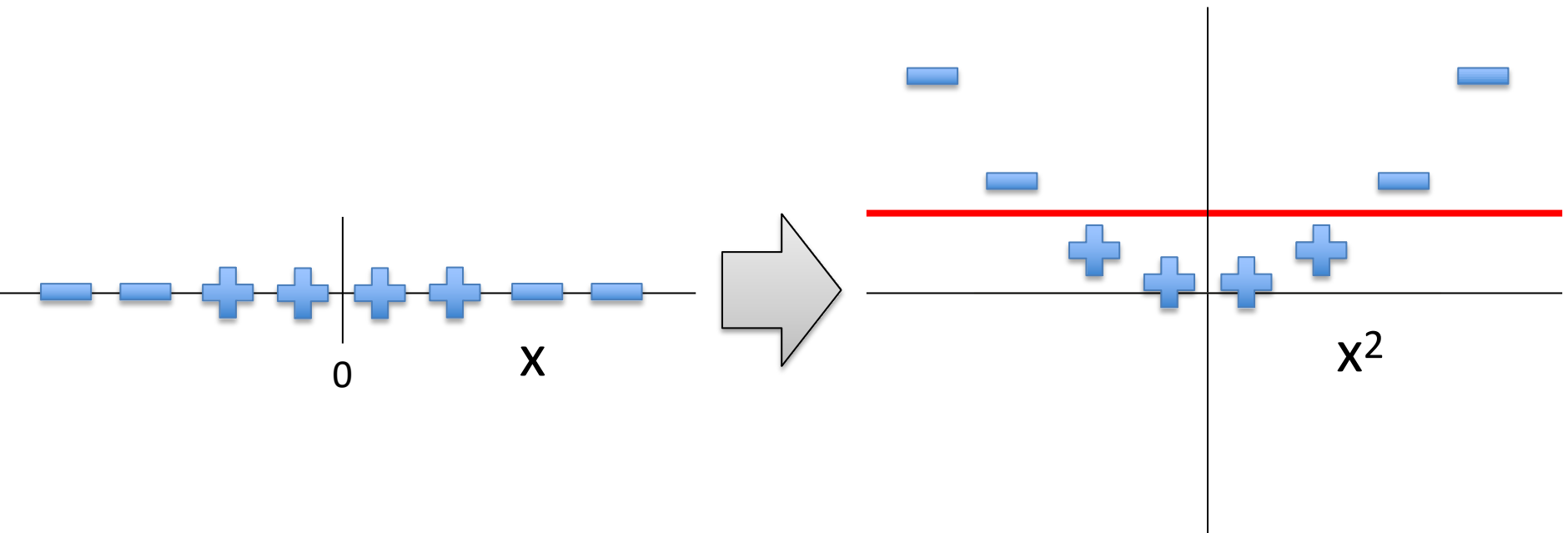


Image from <http://www.atrandomresearch.com/iclass/>

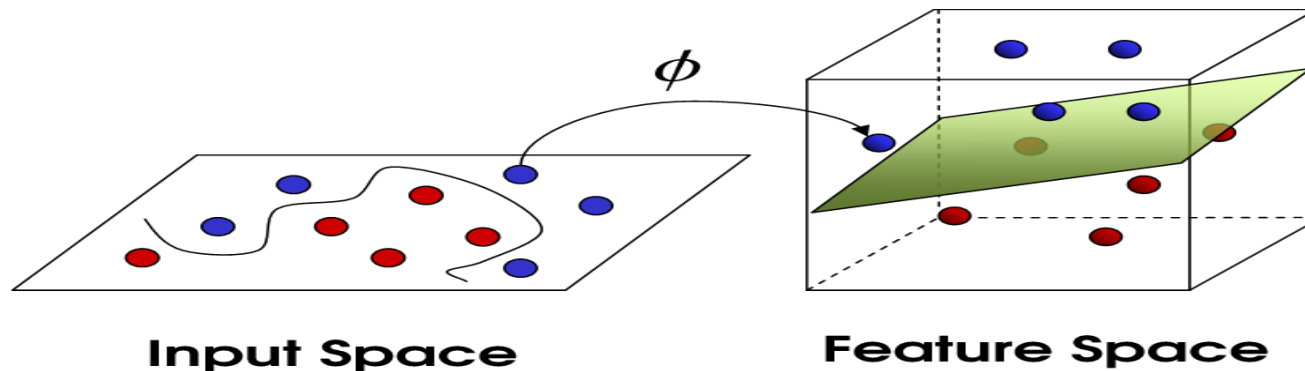
Kernel Methods

Making the Non-Linear Linear

When Linear Separators Fail



Mapping into a New Feature Space



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

- 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 $(\mathbf{x}_i, \mathbf{x}_j)$

The Polynomial Kernel

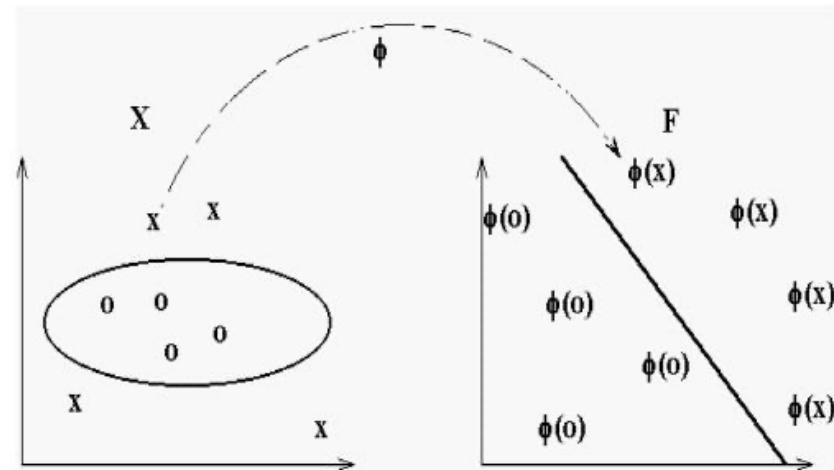
Let $\mathbf{x}_i = [x_{i1}, x_{i2}]$ and $\mathbf{x}_j = [x_{j1}, x_{j2}]$

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

$$\begin{aligned} \Phi(\mathbf{x}_i) &= [x_{i1}^2, x_{j1}^2, \sqrt{2x_{i1}x_{j1}}] \\ \Phi(\mathbf{x}_i) &= [x_{i2}^2, x_{j2}^2, \sqrt{2x_{i2}x_{j2}}] \end{aligned}$$



The Polynomial Kernel

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

Why Kernels are Efficient

The kernel is essentially a function to perform calculations even in the higher dimensions.

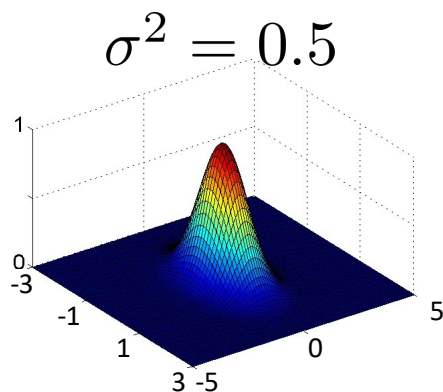
- We use Kernels in SVM to reduce the complexity of calculations.
- A Kernel can do calculations for an even infinite number of dimensions.
 - As the dimensions increase in SVM, it becomes difficult to form a HyperPlane, so we have to resort to Kernels to form a hyperplane.

The Gaussian Kernel

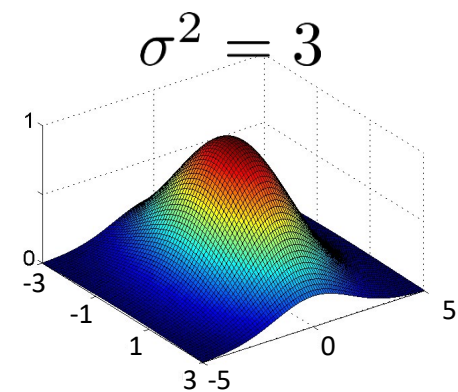
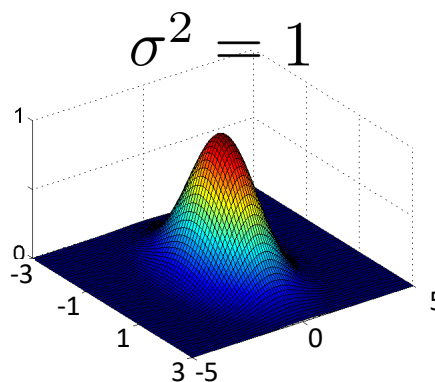
- Also called Radial Basis Function (RBF) kernel

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

- 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

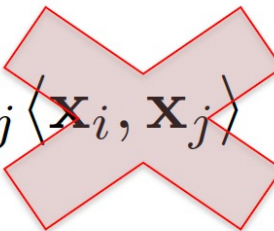


The Kernel Trick

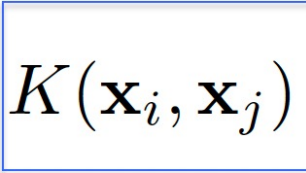
“Given an algorithm which is formulated in terms of a positive definite kernel K_1 , one can construct an alternative algorithm by replacing K_1 with another positive definite kernel K_2 ”

➤ SVMs can use the kernel trick

Incorporating Kernels into SVM

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




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


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

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

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
 - E.g., $K(\mathbf{x}_i, \mathbf{x}_j) = (\langle \mathbf{x}_i, \mathbf{x}_j \rangle + c)^d$
 - $K(\mathbf{x}_i, \mathbf{x}_j) = \exp(-\frac{\|\mathbf{x}_i - \mathbf{x}_j\|_2^2}{2\sigma^2})$

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 $d = 10,000$, $n = 10-1,000$)

- 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

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)