Support Vector Machines & Kernels

Doing *really* well with linear decision surfaces

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Adapted from slides by Tim Oates

One Slide Summary

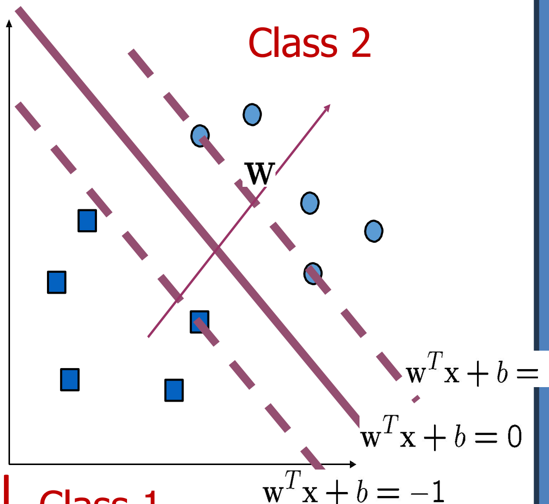
Minimize $\frac{1}{2}\boldsymbol{\theta}^{\top}\boldsymbol{\theta}$
subject to $y_n(\boldsymbol{\theta}^{\top}x_n) \geq 1$, for $n = 1,2,\ldots N$

Maximize Margin
Learn θ (hyperplane)

Minimize **Primal**

$$L(\boldsymbol{\theta},\boldsymbol{\alpha}) = \frac{1}{2}\boldsymbol{\theta}^{\top}\boldsymbol{\theta} - \sum_{i=1}^{n} \alpha_i (y_i(\boldsymbol{\theta}^T x_i) - 1)$$

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



Dual

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

s.t. $\alpha_i \geq 0 \ \forall i$ (comes from Lagrangian Assumptions)

$$\sum_i \alpha_i y_i = 0$$

(comes from differentiating w.r.t θ_0)

Maximize Margin
Learn α (weight
of support vectors)

SVM Dual

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

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

$$\sum_i \alpha_i y_i = 0$$

The decision function is given by

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

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

Interesting Twist: Many α_i's are zero. Only SVs have non-zero α_i's

Understanding the Dual

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

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

$$\sum_i \alpha_i y_i = 0$$

In the solution, either:

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

What if Data Are Not Linearly Separable?

Cannot find $\boldsymbol{\theta}$ that satisfies. $y_i(\theta^T x_i) \geq 1 \; \forall i$

Introduce slack variables ξ_i

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

New Problem

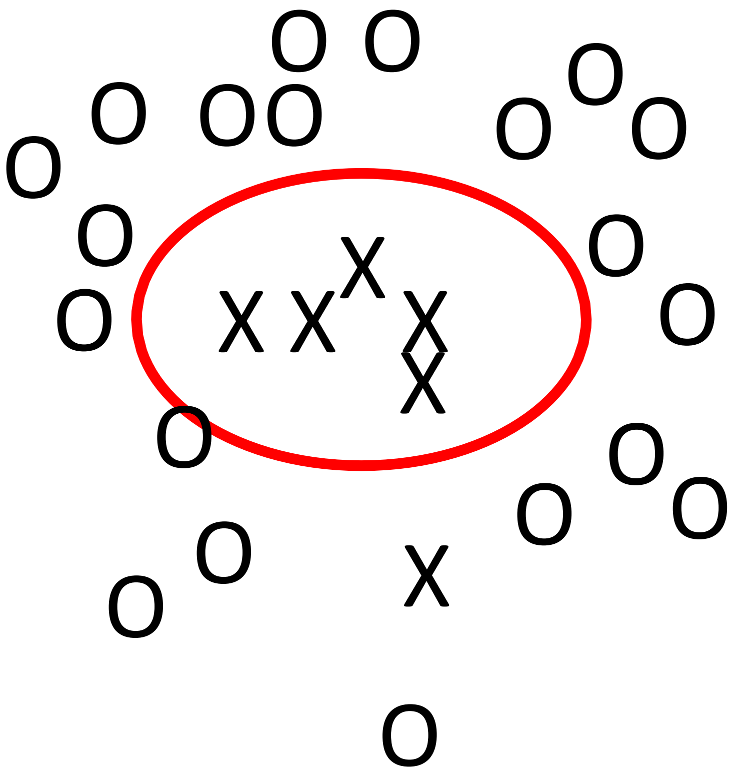
$$\min_{\theta} \frac{1}{2} \sum_{j=1}^{d} \theta_j^2 + C \sum_{i} \xi_i$$

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

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?



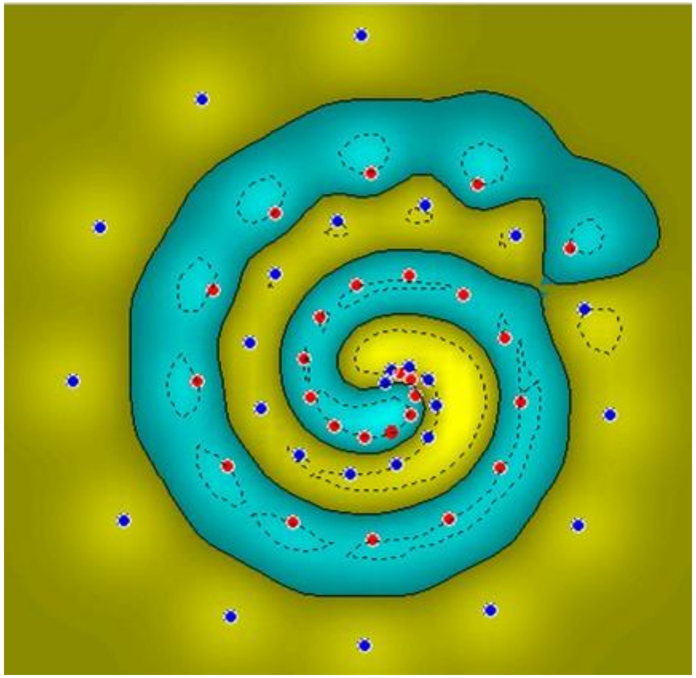
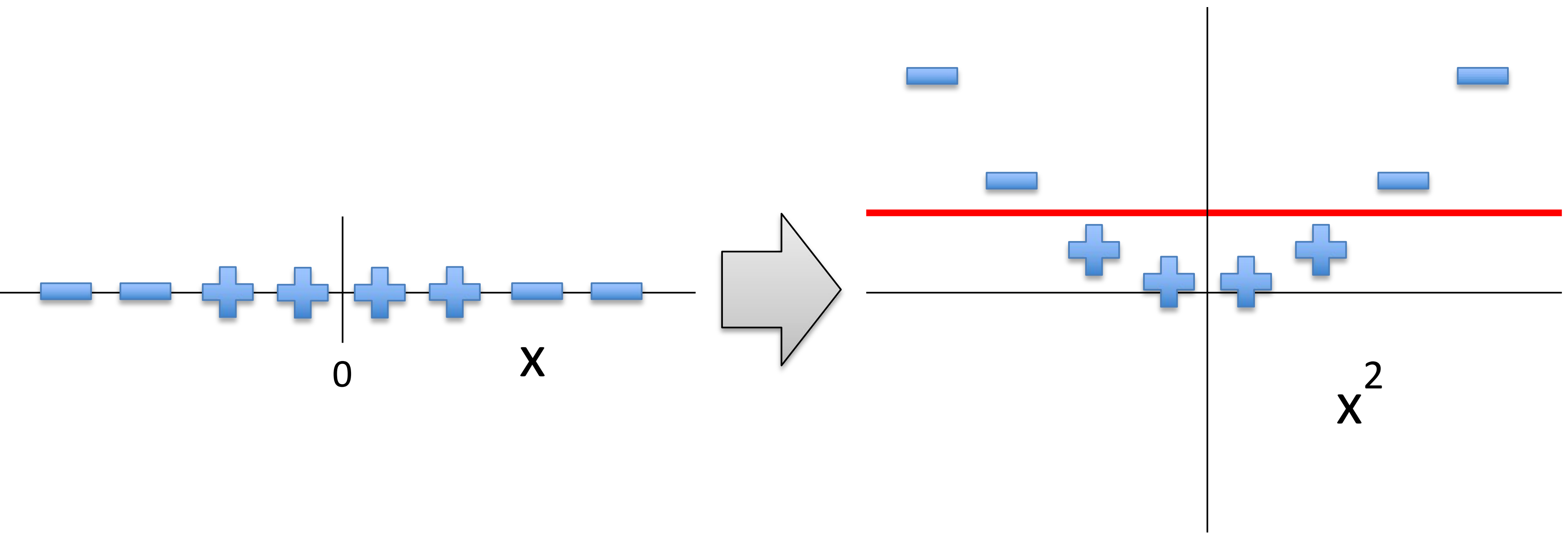


Image from http://www.atrandomresearch.com/iclass/

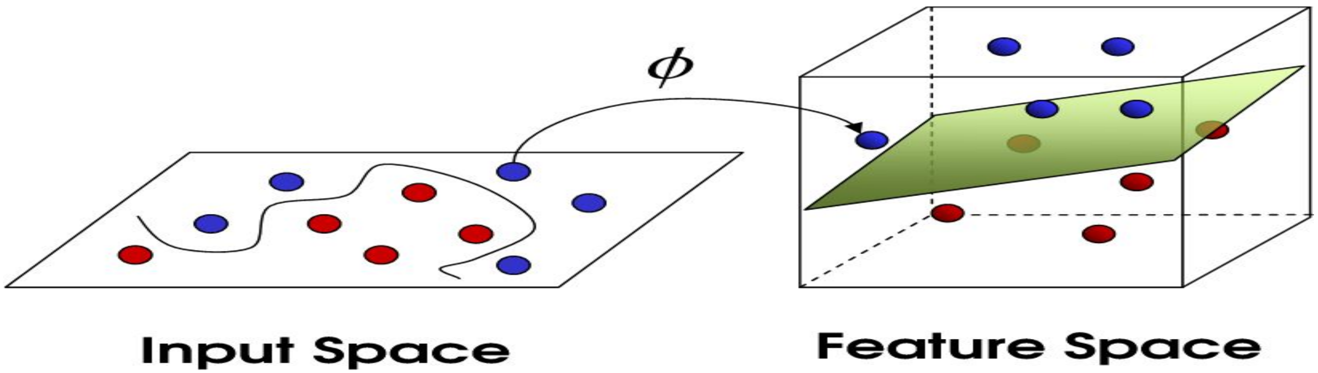
Kernel Methods

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 $\Phi(\mathbf{x}_\mathrm{i})$
  - Find non-linear separator in input space
- What if $\Phi(\mathbf{x}_\mathrm{i})$ 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
$$K(\mathbf{x}_i, \mathbf{x}_j) = \langle \Phi(\mathbf{x}_i), \Phi(\mathbf{x}_j) \rangle$$

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

- Given a function K, it is possible to verify that it is a kernel

Kernel Matrix

- (aka the Gram matrix):

K=

K(1,1)	K(1,2)	K(1,3)	…	K(1,m)
K(2,1)	K(2,2)	K(2,3)	…	K(2,m)
…	…	…	…	…
K(m,1)	K(m,2)	K(m,3)	…	K(m,m)

- The kernel matrix is Symmetric Positive (semi) Definite.
- Any symmetric positive definite matrix can be regarded as a kernel matrix, that is as an inner product matrix in some space

Mercer's Theorem

Every (semi) positive definite, symmetric function is a kernel: i.e. there exists a mapping ϕ s.t. it is possible to write

$$K(x_1, x_2) = \langle \phi(x_1), \phi(x_2) \rangle$$

Positive Definite

$\int K(x,z) f(x) f(z) dx dz \geq 0 , \forall f$ which is square-integrable

More Properties/Kernel Algebra: UMASS CS SVM Lecture Notes

The Polynomial Kernel

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

Consider the following function:

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

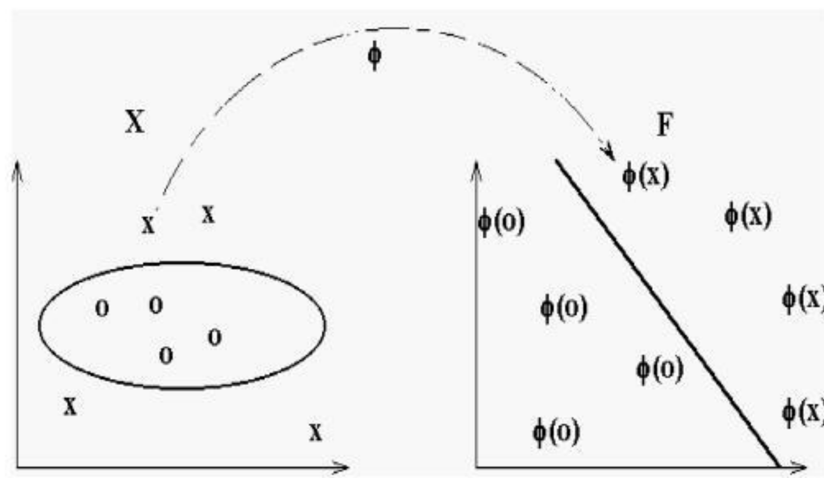
$$= (x_{i1}^2 x_{j1}^2 + x_{i2}^2 x_{j2}^2 + 2x_{i1}x_{i2}x_{j2}x_{j2})$$

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

Where

$$\Phi(\mathbf{x}_i) = [x_{i1}^2, x_{j1}^2, x_{i1}x_{j1}, x_{j1}x_{i1}]$$

$$\Phi(\mathbf{x}_i) = [x_{i2}^2, x_{j2}^2, x_{i2}x_{j2}, x_{j2}x_{i2}]$$



Problems with Feature Space

- Working in high dimensional feature spaces solves the problem of expressing complex functions

But:

- There is a computational problem (working with very large vectors)
- And a generalization theory problem (curse of dimensionality)

The Polynomial Kernel

- Given by $K(\mathbf{x}_i, \mathbf{x}_j) = \langle \mathbf{x}_i, \mathbf{x}_j \rangle^d$
  - Φ(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 Φ(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.

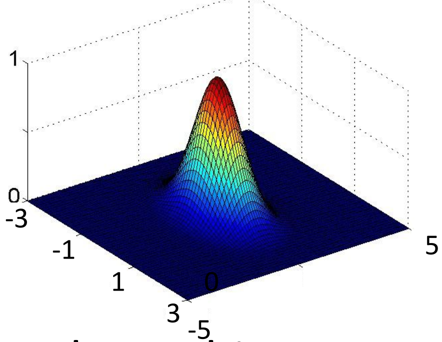
The Gaussian Kernel

- Also called Radial Basis Function (RBF) kernel

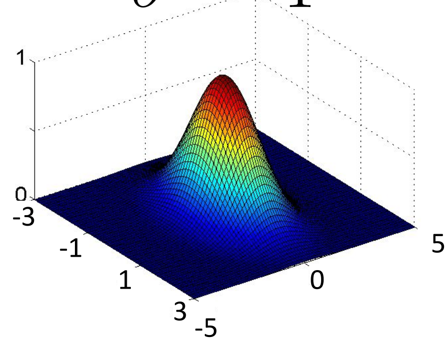
$$K(\mathbf{x}_i, \mathbf{x}_j) = \exp\left(-\frac{\|\mathbf{x}_i - \mathbf{x}_j\|_2^2}{2\sigma^2}\right)$$

  - Has value 1 when $x_i = x_j$
  - Value falls off to 0 with increasing distance
  - Note: Need to do feature scaling <u>before</u> using Gaussian Kernel

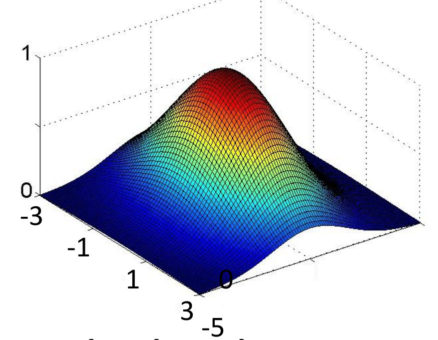
$\sigma^2 = 0.5$



$\sigma^2 = 1$



$\sigma^2 = 3$



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

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

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

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

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

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

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)