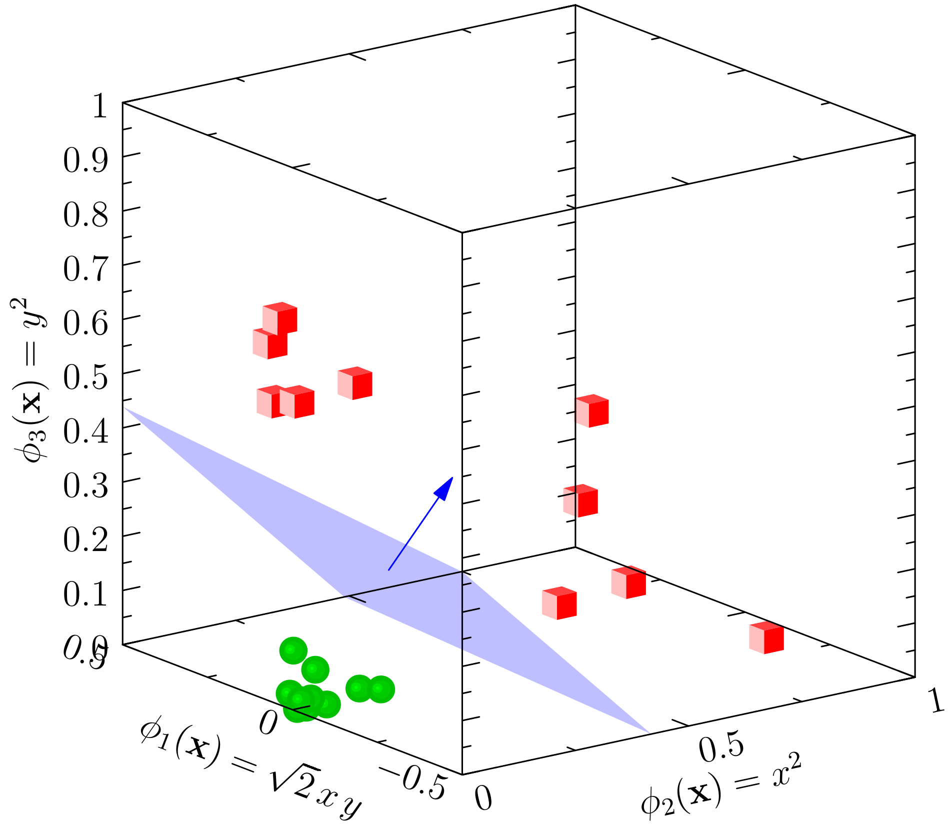
Advanced Machine Learning

Support Vector Machines



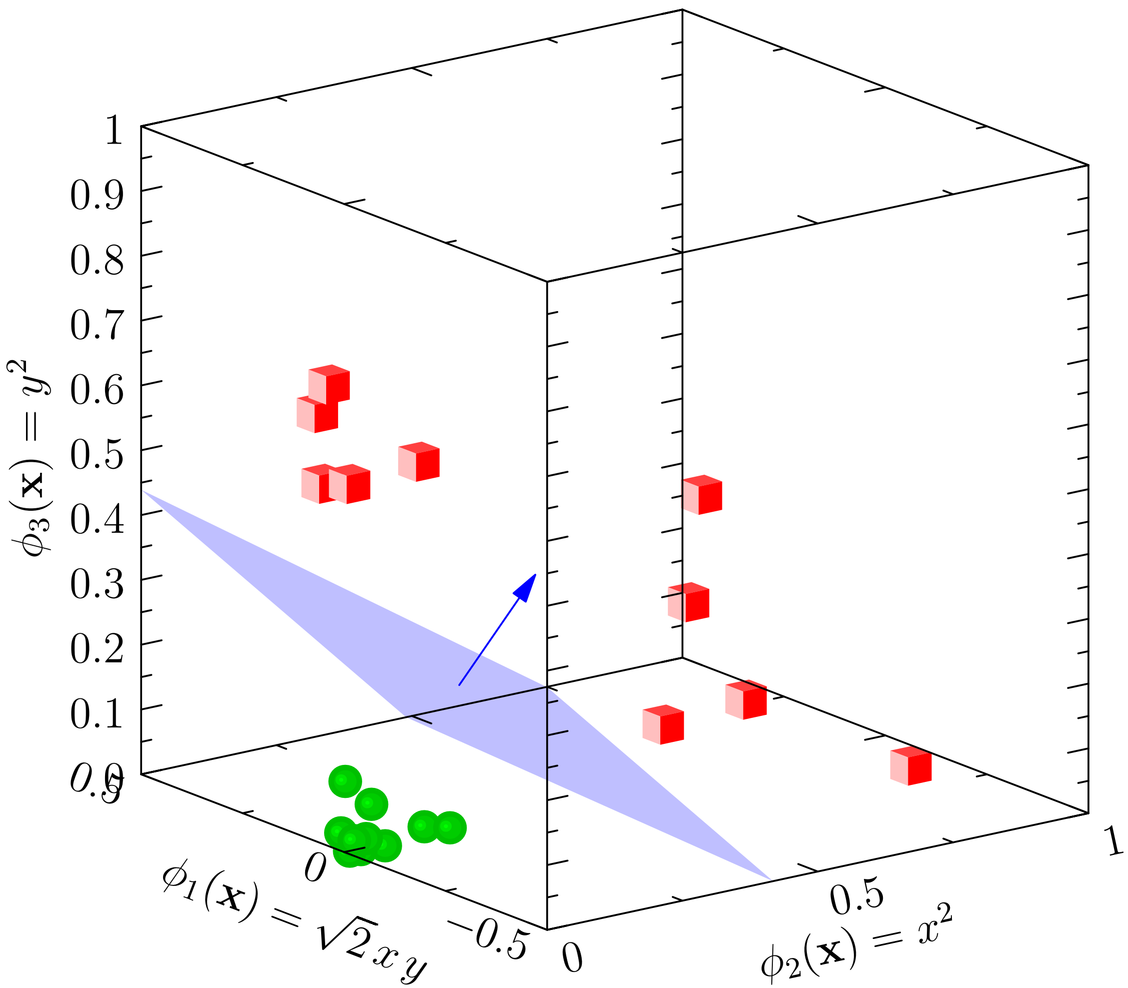
Support Vector Machines, maximum margins

Outline

1. **The Big Picture**

2. Practice

3. Maximum Margins

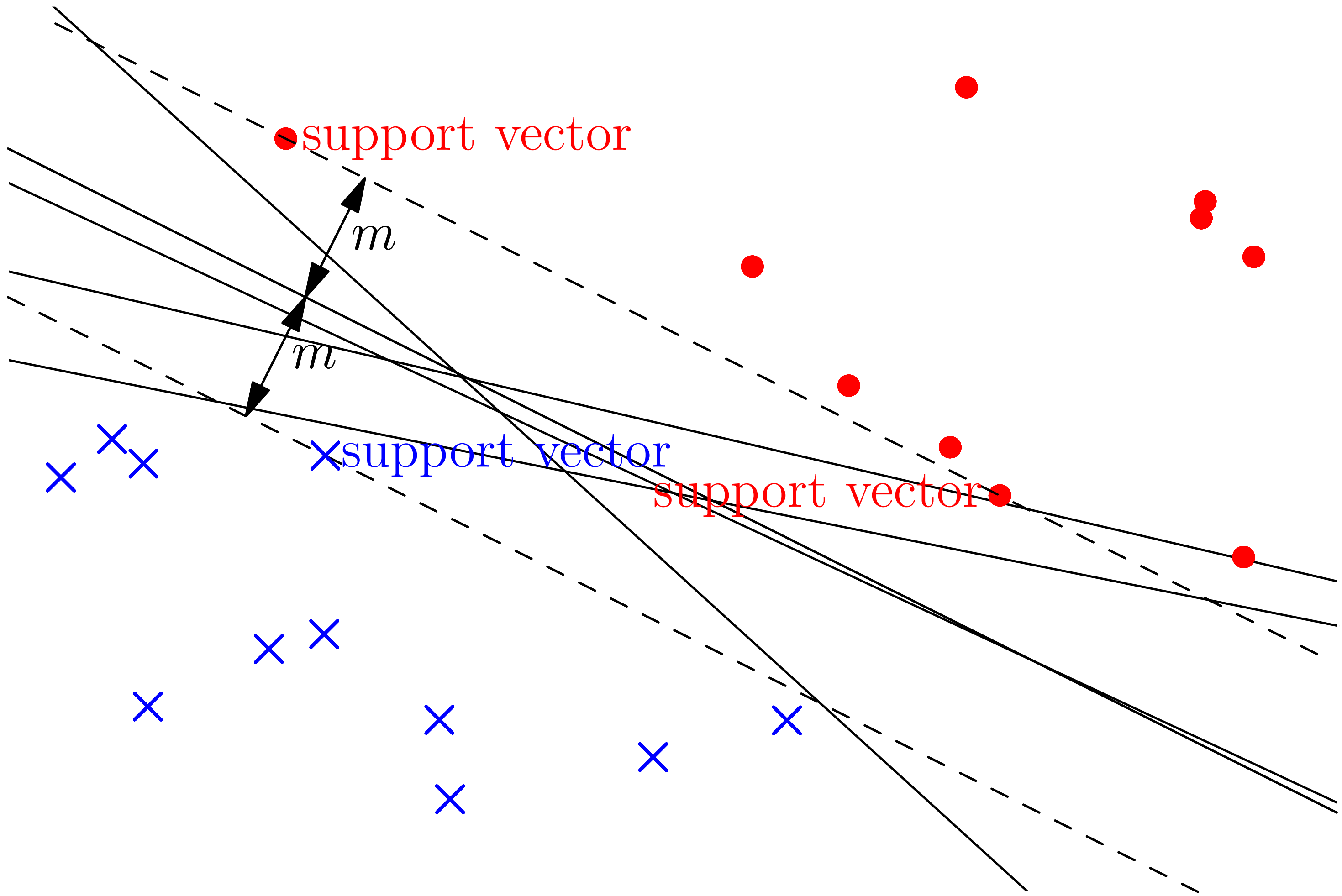


Support Vector Machines

- Support vector machines, when used right, often have the best generalisation results
- They are typically used on numerical data, but can and have been adapted to text, sequences, etc.
- Although not as trendy as deep learning, they will often be the method of choice on small data sets
- They subtly regularise themselves, choosing a solution that generalises well from a host of different solutions

Linear Separation of Data

- SVMs classify linearly separable data



- Finds maximum-margin separating plane

Extended Feature Space

- To increase the likelihood of linear-separability we often use a high-dimensional mapping

$$\boldsymbol{x} = (x_1, x_2, \ldots, x_p) \to \vec{\phi}(\boldsymbol{x}) = (\phi_1(\boldsymbol{x}), \phi_2(\boldsymbol{x}), \ldots, \phi_m(\boldsymbol{x}))$$

$m \gg p$

- Finding the maximum margin hyper-plane is time consuming in "primal" form if m is large

- We can work in the "dual" space of patterns, then we only need to compute dot products

$$\vec{\phi}(\boldsymbol{x}_i) \cdot \vec{\phi}(\boldsymbol{x}_j) = \sum_{k=1}^{m} \phi_k(\boldsymbol{x}_i)\, \phi_k(\boldsymbol{x}_j)$$

Kernel Trick

- If we choose a **positive semi-definite** kernel function $K(\boldsymbol{x}, \boldsymbol{y})$ then there exists functions $\phi_k(\boldsymbol{x})$, such that

$$K(\boldsymbol{x}_i, \boldsymbol{x}_j) = \vec{\phi}(\boldsymbol{x}_i) \cdot \vec{\phi}(\boldsymbol{x}_j)$$

  (like an eigenvector decomposition of a matrix)

- Never need to compute $\phi_k(\boldsymbol{x}_i)$ explicitly as we only need the dot-product $\vec{\phi}(\boldsymbol{x}_i) \cdot \vec{\phi}(\boldsymbol{x}_j) = K(\boldsymbol{x}_i, \boldsymbol{x}_j)$ to compute maximum margin separating hyper-plane

- Sometimes $\vec{\phi}(\boldsymbol{x}_i)$ is an infinite dimensional vector so its good we don't have to compute it!

Kernel Functions

- Kernel functions are symmetric functions of two variable
- Strong restriction: *positive semi-definite*
- Examples

$$\text{Quadratic kernel:} \qquad K(\boldsymbol{x}_1, \boldsymbol{x}_2) = \left(\boldsymbol{x}_1^{\mathsf{T}} \boldsymbol{x}_2\right)^2$$

$$\text{Gaussian (RBF) kernel:} \qquad K(\boldsymbol{x}_1, \boldsymbol{x}_2) = \mathrm{e}^{-\gamma \, \|\boldsymbol{x}_1 - \boldsymbol{x}_2\|^2}$$

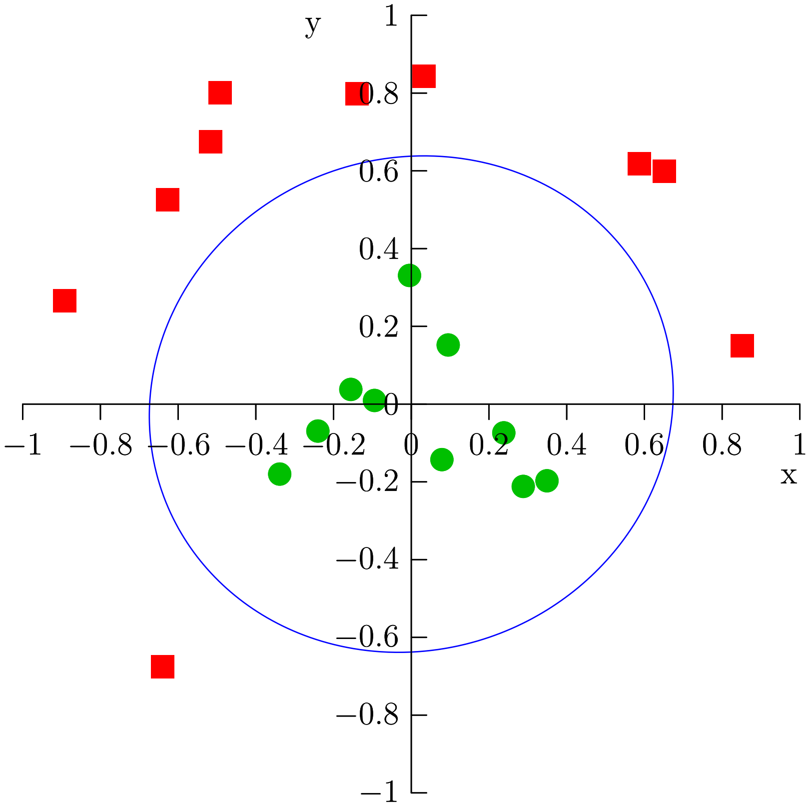
- Consider the mapping

$$\boldsymbol{x}_i = \begin{pmatrix} x_i \\ y_i \end{pmatrix} \rightarrow \boldsymbol{\phi}(\boldsymbol{x}_i) = \begin{pmatrix} x_i^2 \\ y_i^2 \\ \sqrt{2}\, x_i\, y_i \end{pmatrix}$$

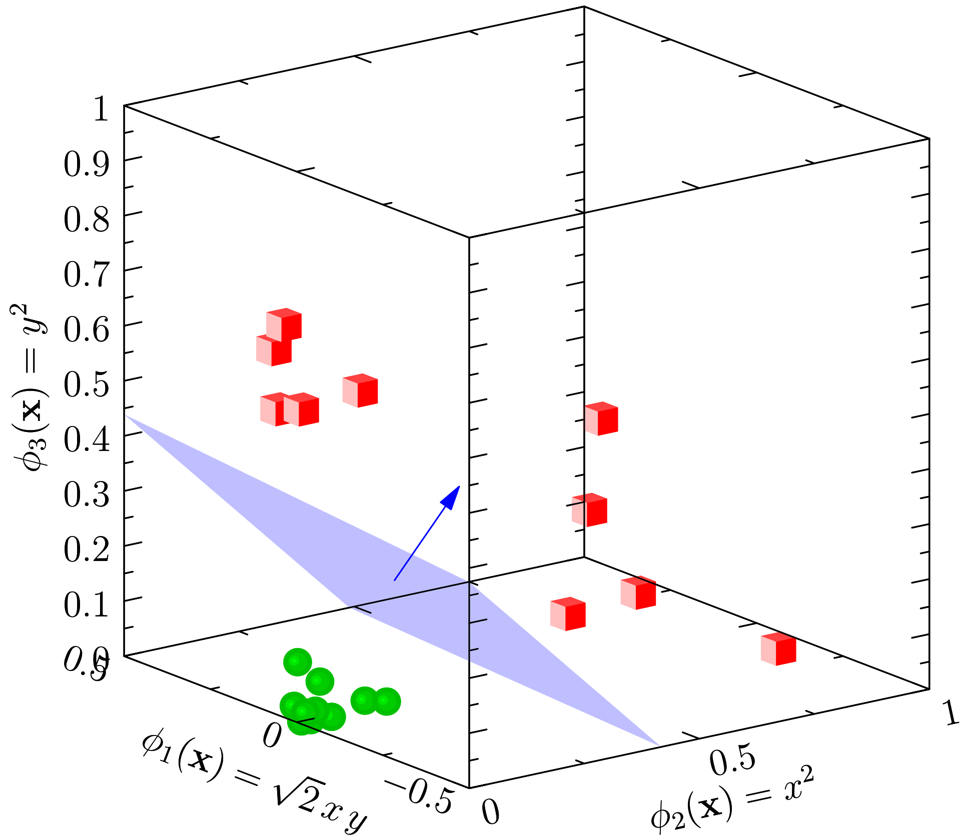
Non-linearly Separation of Data

$$K(\boldsymbol{x}_1,\,\boldsymbol{x}_2) = \begin{pmatrix} x_1^2 & y_1^2 & \sqrt{2}\,x_1\,y_1 \end{pmatrix} \begin{pmatrix} x_2^2 \\ y_2^2 \\ \sqrt{2}\,x_2\,y_2 \end{pmatrix} = x_1^2\,x_2^2 + y_1^2\,y_2^2 + 2\,x_1\,y_1\,x_2\,y_2$$

$$= (x_1\,x_2 + y_1\,y_2)^2 = \left(\boldsymbol{x}_1^T \boldsymbol{x}_2\right)^2$$

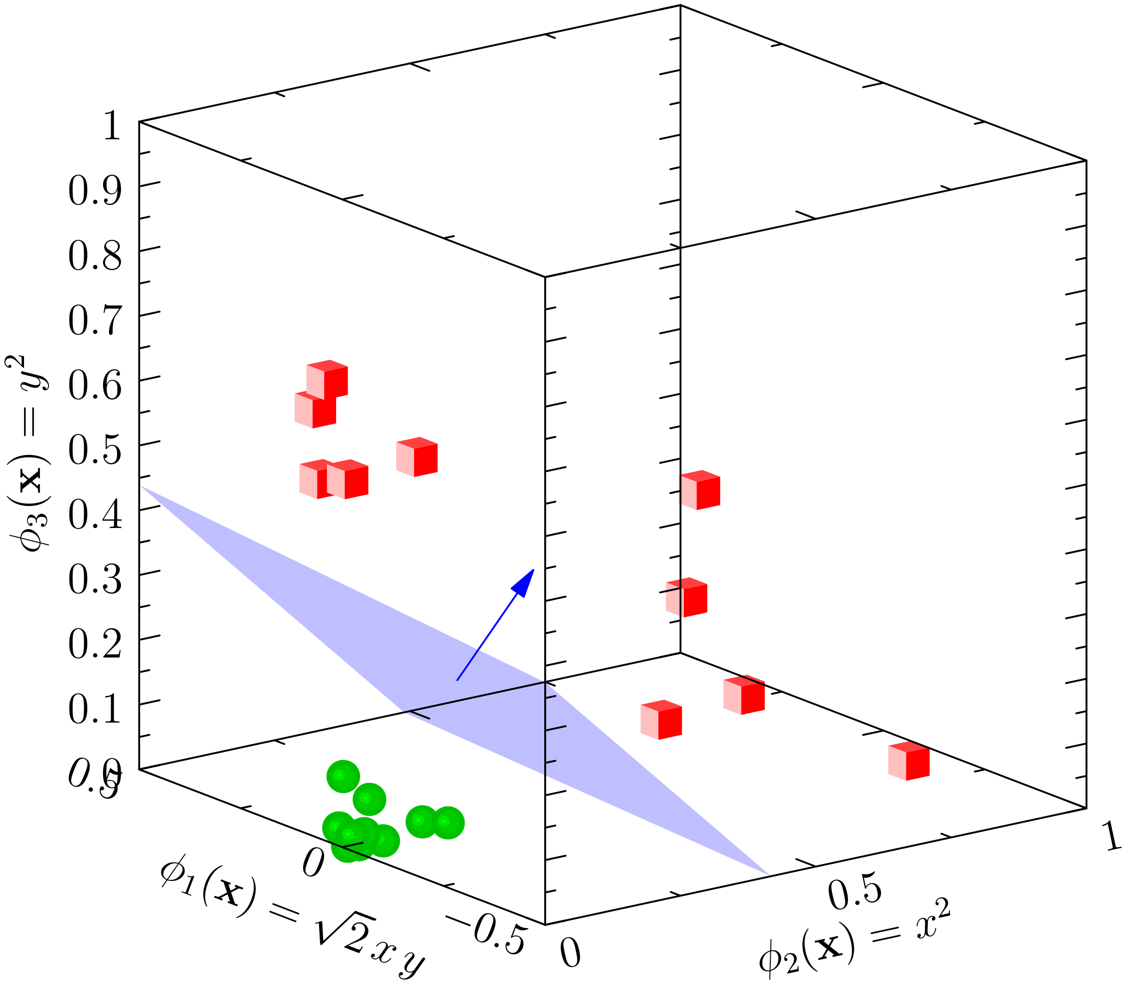


$$\xrightarrow{\boldsymbol{x} \to \boldsymbol{\phi}(\boldsymbol{x})}$$



Outline

1. The Big Picture
2. **Practice**
3. Maximum Margins

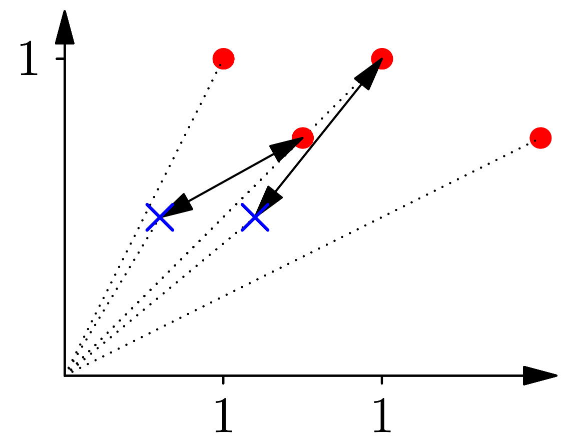


Computing the Maximum-Margin Hyper-plane

- We will derive the formula for the minimum-margin hyper-plane in the next lecture
- This gives us a quadratic programming problem
- Through a neat trick we can represent this problem in a "dual form" where we
- Never need to compute $\boldsymbol{\phi}_i(\boldsymbol{x})$ only need to compute $K(\boldsymbol{x}_i, \boldsymbol{x}_j)$
- When we use the kernel trick the time to compute the solution to the quadratic programming problem is $p\,N^3$ where N is the number of training examples and p is the number of features

Getting SVMs to Work Well

- SVMs rely on distances between data points
- These will change relative to each other if we rescale some features but not other—giving different maximum-margin hyper-planes

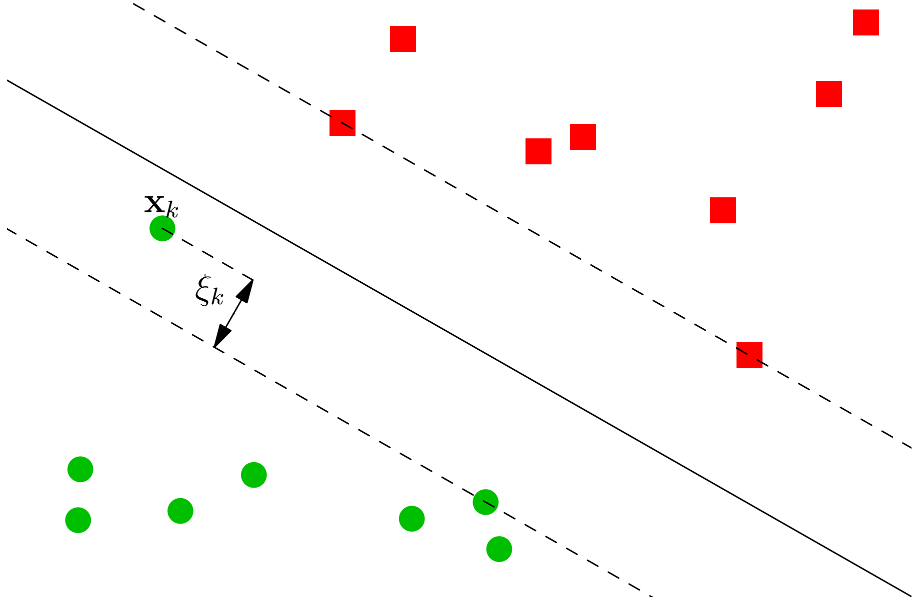


- If we don't know what features are important (most often the case), then it is worth scaling each feature (for example, so their range is between 0 and 1 or their variance is 1)

Soft Margins

- Sometimes the margin constraint is too severe
- Relax constraints by introducing *slack variables*, $\xi_k \geq 0$

$$y_k(\boldsymbol{x}_k^\mathsf{T}\boldsymbol{w} - b) \geq 1 - \xi_k$$



- Minimise $\frac{\|\boldsymbol{w}\|^2}{2} + C\sum_{k=1}^{n} \xi_k$ subject to constraints
- Large C punishes slack variables

Optimising C

- In practice it can make a huge difference to the performance if we change C
- Optimal C values changes by many orders of magnitude e.g. 2^{-5}–2^{15}
- Typically optimised by a grid search (start from 2^{-5} say and double until you reach 2^{15})

Choosing the Right Kernel Function

- There are kernels design for particular data types (e.g. string kernels for text or biological sequences)

- For numerical data people tend to look at using no kernel (linear SVM), a radial basis function (Gaussian) kernel or polynomial kernels

- Kernel's often come with parameters, e.g. the popular radial basis function kernel

$$K(\boldsymbol{x}, \boldsymbol{y}) = \mathrm{e}^{-\gamma \, \|\boldsymbol{x}-\boldsymbol{y}\|^2}$$

- Optimal γ values range over 2^{-15}–2^{3}

SVM Libraries

- Although SVMs have unique solutions, they require very well written optimisers
- If you have a large data set they can be very slow
- There are good libraries out there, svmlib, svm-lite, etc.
- These will often automate normalisation of data and grid search for parameters

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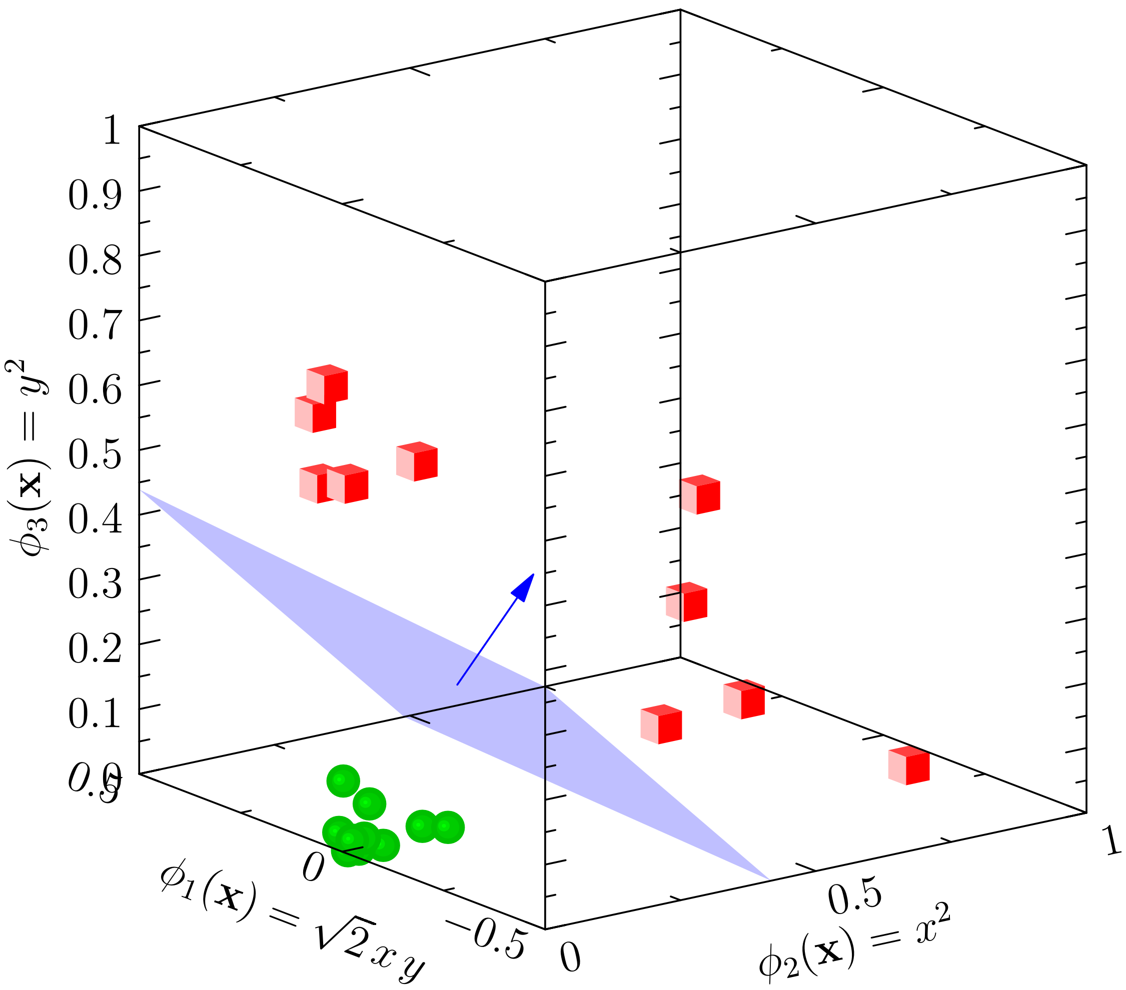
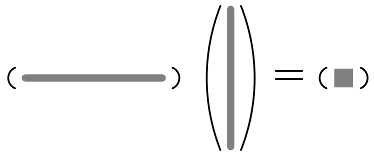


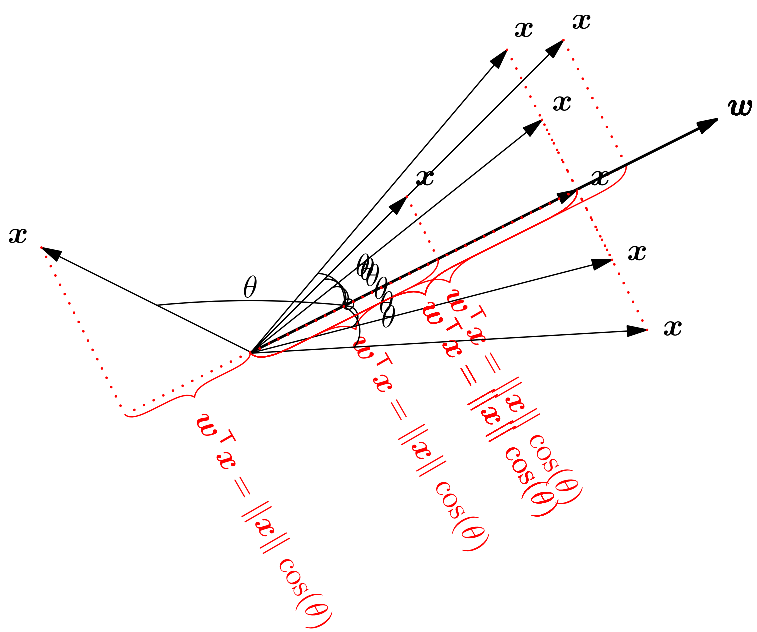
Dot Product

- Recall the dot product



$$\boldsymbol{x} \cdot \boldsymbol{y} = \boldsymbol{x}^\mathsf{T} \boldsymbol{y} = \sum_{i=1}^{n} x_i \, y_i = \|\boldsymbol{x}\| \, \|\boldsymbol{y}\| \, \cos(\theta)$$

- If $\|\boldsymbol{w}\| = 1$ then $\boldsymbol{x}^\mathsf{T} \boldsymbol{w} = \|\boldsymbol{x}\| \, \cos(\theta)$



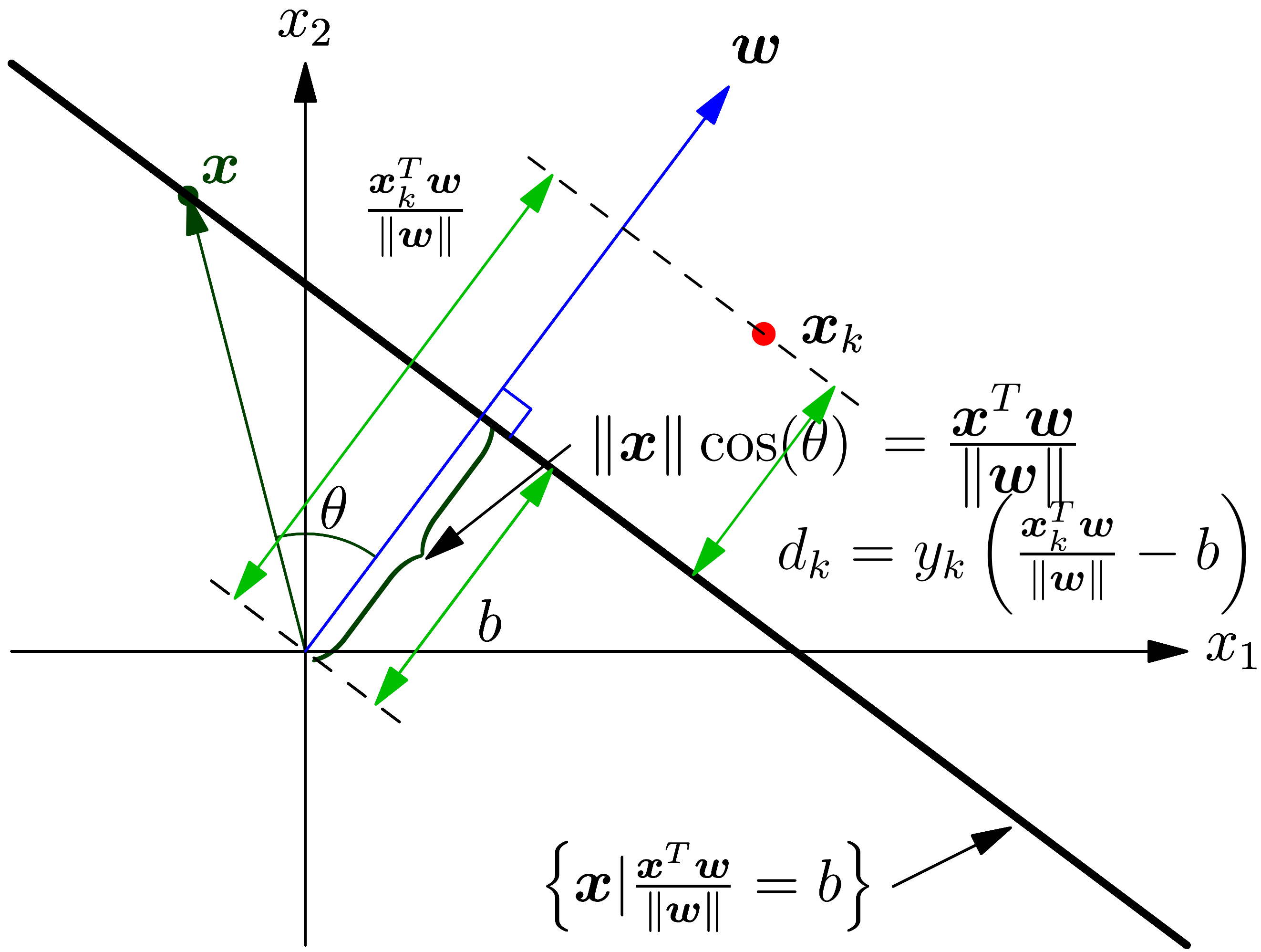
Maximise Margin

- Consider a linearly separable set of data
  - ⋆ $\mathcal{D} = \{(\boldsymbol{x}_k, y_k)\}_{k=1}^{P}$
  - ⋆ $y_k \in \{-1, 1\}$
- Our task is to find a separating plane defined by the orthogonal vector $\boldsymbol{w}$ and a threshold b such that

$$y_k \left(\frac{\boldsymbol{w}^\mathsf{T} \boldsymbol{x}_k}{\|\boldsymbol{w}\|} - b \right) \geq m$$

where m is the margin

Distance to hyperplanes



Constrained Optimisation

- Wish to find $\boldsymbol{w}$ and b to maximise m subject to constraints

$$y_k \left(\frac{\boldsymbol{w}^\mathsf{T} \boldsymbol{x}_k}{\|\boldsymbol{w}\|} - b \right) \geq m \quad \text{for all } k = 1, 2, \ldots, P$$

- If we divide through by m

$$y_k \left(\frac{\boldsymbol{w}^\mathsf{T} \boldsymbol{x}_k}{m\,\|\boldsymbol{w}\|} - \frac{b}{m} \right) \geq 1 \quad \text{for all } k = 1, 2, \ldots, P$$

- Define $\hat{\boldsymbol{w}} = \boldsymbol{w}/(m\|\boldsymbol{w}\|)$ and $\hat{b} = b/m$

$$y_k \left(\hat{\boldsymbol{w}}^\mathsf{T} \boldsymbol{x}_k - \hat{b} \right) \geq 1$$

Quadratic Programming Problem

- Note that as $\hat{\boldsymbol{w}} = \boldsymbol{w}/(m\|\boldsymbol{w}\|)$

$$\|\hat{\boldsymbol{w}}\| = \left\| \frac{\boldsymbol{w}}{m\,\|\boldsymbol{w}\|} \right\| = \frac{1}{m}$$

- Minimising $\|\hat{\boldsymbol{w}}\|^2$ is equivalent to maximising the margin m

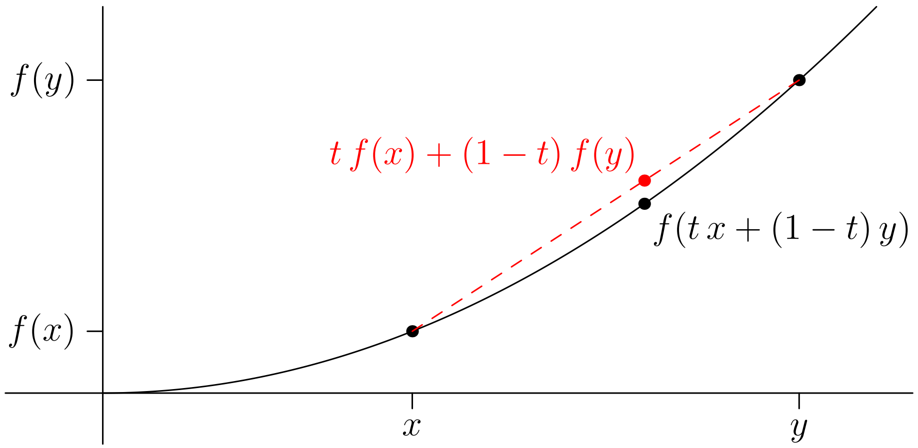
- Can write the optimisation problem as a *quadratic programming problem*

$$\min_{\hat{\boldsymbol{w}},\,\hat{b}} \frac{\|\hat{\boldsymbol{w}}\|^2}{2} \quad \text{subject to } y_k\left(\hat{\boldsymbol{w}}^{\mathsf{T}}\boldsymbol{x}_k - \hat{b}\right) \geq 1 \text{ for all } k = 1,\, 2,\, \ldots,\, P$$

Convexity

- The quadratic function $f(x) = x^2$ is an example of a *convex* function satisfying

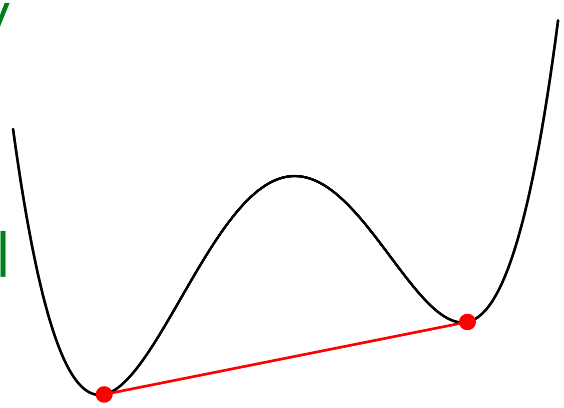
$$f(tx + (1-t)y) \leq t f(x) + (1-t) f(y) \quad \text{for } 0 \leq t \leq 1$$



- This extends to high dimensions
$$f(t\boldsymbol{x} + (1-t)\boldsymbol{y}) \leq t f(\boldsymbol{x}) + (1-t) f(\boldsymbol{y})$$

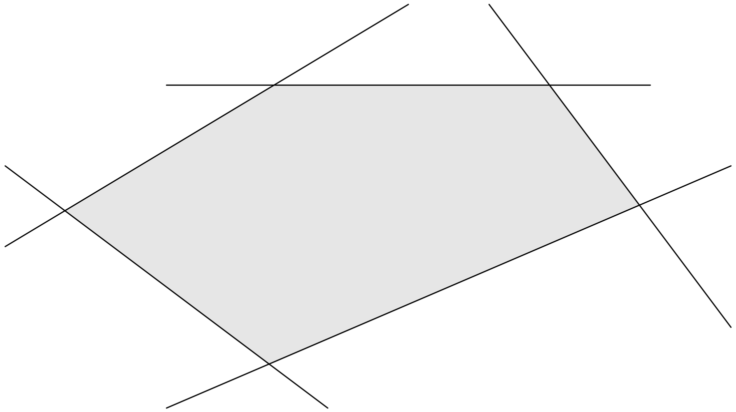
Unique Minimum

- Convex function have a unique minimum
- The existence of a local minimum would break convexity
  - ⋆ The line connecting a local minimum to a global minimum would be strictly decreasing
  - ⋆ Thus there are points next to the local minimum with lower values
  - ⋆ This is a contradiction



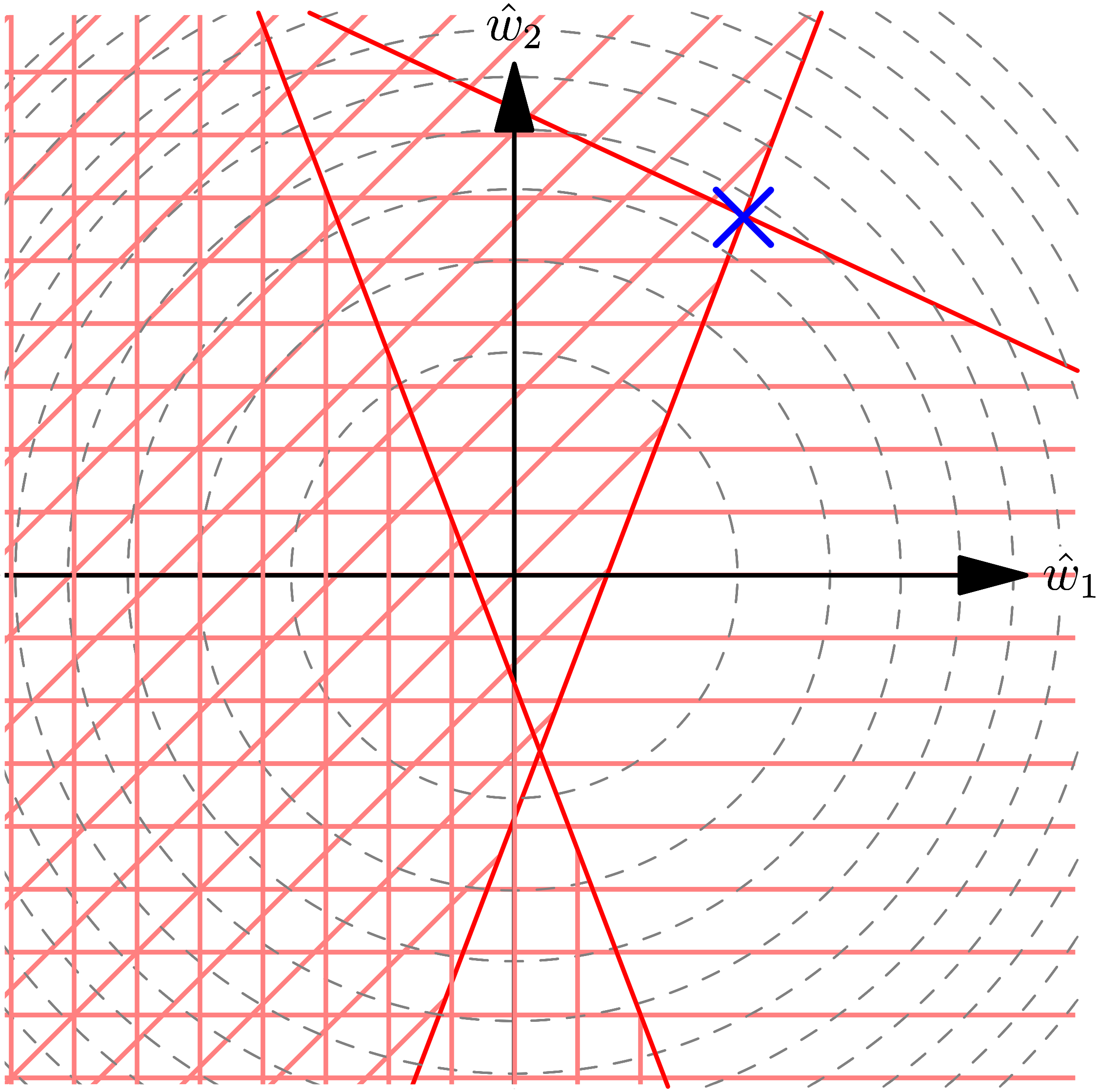
- This remains true if we consider convex functions that a constrained to live in a **convex region**

Convex Regions



- Convex regions are familiar
- Convex function constrained to lie in a convex region will also have unique minima as minima can't hide in corners unlike concave regions
- Quadratic programming problems involving a quadratic function and linear constraints are convex and have a unique minimum

Quadratic Programming in SVMs



Quadratic Programming

- We have a quadratic programming problem for the weights $\hat{\boldsymbol{w}} = (\hat{w}_1, \hat{w}_2, \ldots, \hat{w}_n)$ and bias b and P constraints

- This is a classic but fiddly optimisation problems

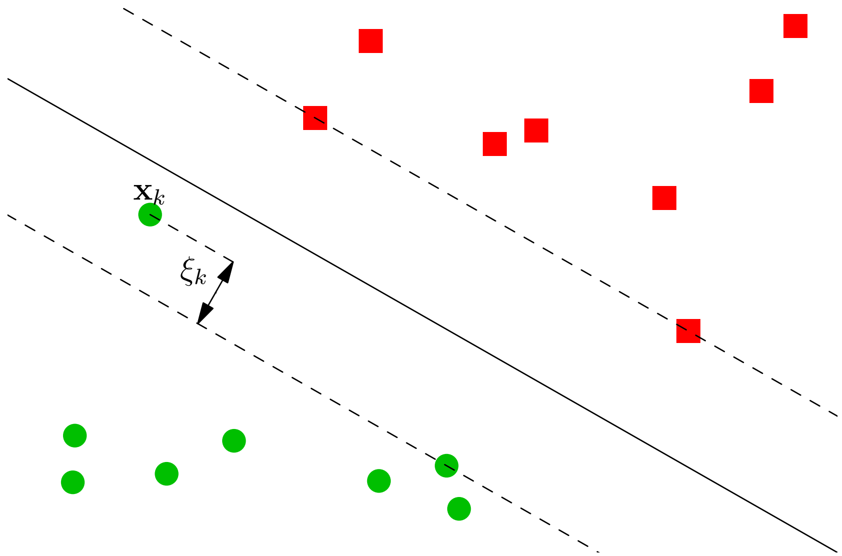
- It can be solved in $O(n^3)$ time (it involves inverting matrices) (phew it is not NP-complete!)

- We will see that there is an equivalent dual problem which allows us to use the kernel trick

Soft Margins

- Can relax constraints by introducing *slack variables*, $\xi_k \geq 0$

$$y_k(\hat{\boldsymbol{w}}^\mathsf{T}\boldsymbol{x}_k - \hat{b}) \geq 1 - \xi_k$$



- Minimise $\frac{\|\hat{\boldsymbol{w}}\|^2}{2} + C\sum_{k=1}^{n} \xi_k$ subject to constraints

- We've added a linear function that leaves our objective convex

Convexity of Lasso

- Recall that in Lasso we are asked to minimise

$$E = \sum_{n=1}^{N} \left(\boldsymbol{w}^{\mathsf{T}} \boldsymbol{x}_n - y_n \right)^2 + \nu \sum_{i=1}^{p} |w_i|$$

- We can rewrite this (using $w_i = w_i^+ - w_i^-$) as

$$E = \sum_{n=1}^{N} \left((\boldsymbol{w}^+ - \boldsymbol{w}^-)^{\mathsf{T}} \boldsymbol{x}_n - y_n \right)^2 + \nu \sum_{i=1}^{p} (w_i^+ + w_i^-)$$

$$\text{subject to} \quad w_i^+, w_i^- \geq 0 \quad \text{for all } i$$

- Again it Lasso has a unique minima

Conclusions

- We've seen how SVMs work
- We've learnt how to use them
- We've seen that we can find the maximum margin hyper-plane by solving a quadratic programming problem (with a unique solution)
- This is a convex optimisation problem with a unique optimum
- Next we will look at the **dual problem**