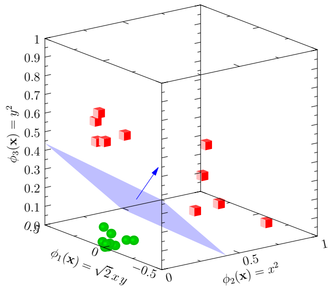
Advanced Machine Learning

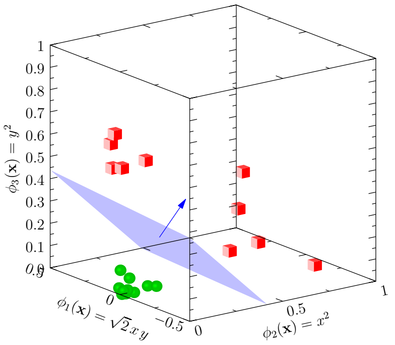
Support Vector Machines



Support Vector Machines, maximum margins

Outline

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

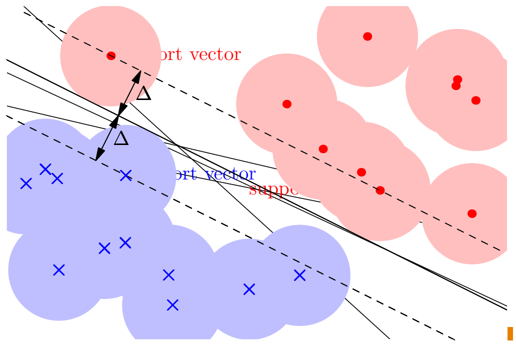


Support Vector Machines

- 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

$$\boldsymbol{x} = (x_1, x_2, \ldots, x_p)^{\mathsf{T}} \to \boldsymbol{\phi}(\boldsymbol{x}) = (\phi_1(\boldsymbol{x}), \phi_2(\boldsymbol{x}), \ldots, \phi_r(\boldsymbol{x}))^{\mathsf{T}}$$

$r \gg p$

- Finding the maximum margin hyper-plane is time consuming in "primal" form if r is large
- We can work in the "dual" space of patterns, then we only need to compute inner-products

$$\langle \boldsymbol{\phi}(\boldsymbol{x}_i), \boldsymbol{\phi}(\boldsymbol{x}_j) \rangle = \boldsymbol{\phi}(\boldsymbol{x}_i)^{\mathsf{T}} \boldsymbol{\phi}(\boldsymbol{x}_j) = \sum_{k=1}^{r} \phi_k(\boldsymbol{x}_i)\phi_k(\boldsymbol{x}_j)$$

Kernel Trick

- If we choose a **positive semi-definite** kernel function $K(\boldsymbol{x}, \boldsymbol{y})$ then there exists functions $\boldsymbol{\phi}(\boldsymbol{x}) = (\phi_k(\boldsymbol{x}) | k = 1, 2, \ldots, r)$, such that

$$K(\boldsymbol{x}_i, \boldsymbol{x}_j) = \langle \boldsymbol{\phi}(\boldsymbol{x}_i), \boldsymbol{\phi}(\boldsymbol{x}_j) \rangle$$

(like an eigenvector decomposition of a matrix)

- Never need to compute $\phi_k(\boldsymbol{x}_i)$ explicitly as we only need the inner-product $\langle \boldsymbol{\phi}(\boldsymbol{x}_i), \boldsymbol{\phi}(\boldsymbol{x}_j) \rangle = K(\boldsymbol{x}_i, \boldsymbol{x}_j)$ to compute maximum margin separating hyper-plane
- Sometimes $\boldsymbol{\phi}(\boldsymbol{x}_i)$ is an infinite dimensional vector so it is good we don't have to compute all the elements!

Kernel Functions

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

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

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

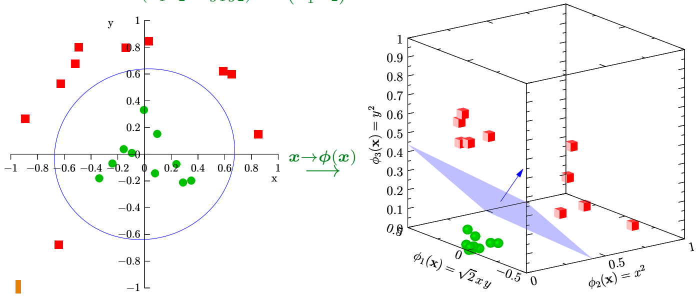
- Consider the mapping

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

Non-linear Separation of Data

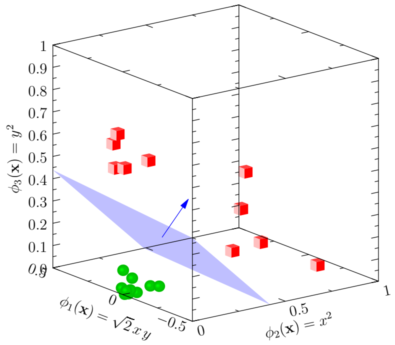
$$K(\boldsymbol{x}_1, \boldsymbol{x}_2) = \begin{pmatrix} x_1^2 & y_1^2 & \sqrt{2}x_1 y_1 \end{pmatrix} \begin{pmatrix} x_2^2 \\ y_2^2 \\ \sqrt{2}x_2 y_2 \end{pmatrix} = x_1^2 x_2^2 + y_1^2 y_2^2 + 2 x_1 y_1 x_2 y_2$$

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



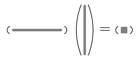
Outline

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



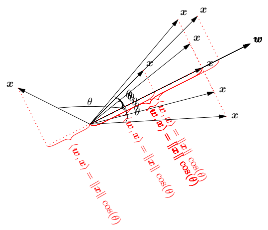
Inner Product

- Recall the inner or dot product in $\mathbb{R}^n$



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

- If $\|\boldsymbol{w}\| = 1$ then $\langle \boldsymbol{x}, \boldsymbol{w} \rangle = \|\boldsymbol{x}\| \cos(\theta)$



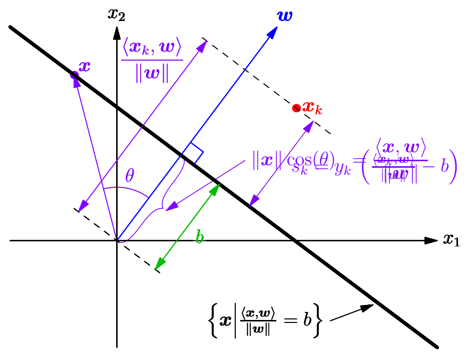
Maximise Margin

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

$$y_k \left(\frac{\langle \boldsymbol{w}, \boldsymbol{x}_k \rangle}{\|\boldsymbol{w}\|} - b \right) \geq \Delta$$

where Δ is the margin

Distance to hyperplanes



Constrained Optimisation

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

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

- If we divide through by Δ

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

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

$$y_k \left(\langle \hat{\boldsymbol{w}}, \boldsymbol{x}_k \rangle - \hat{b} \right) \geq 1$$

Quadratic Programming Problem

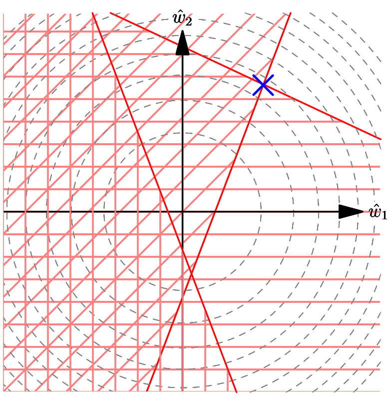
- Note that as $\hat{\boldsymbol{w}} = \boldsymbol{w} / (\Delta \|\boldsymbol{w}\|)$

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

- Minimising $\|\hat{\boldsymbol{w}}\|^2$ is equivalent to maximising the margin Δ
- Can write the optimisation problem as a *quadratic programming problem*

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

Quadratic Programming in SVMs

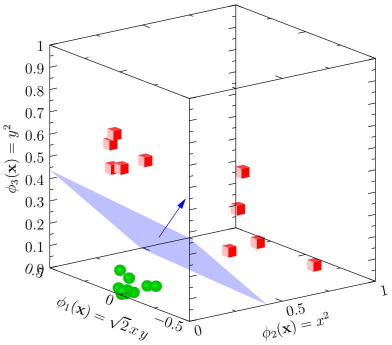


Quadratic Programming

- We have a quadratic programming problem for the weights $\hat{\boldsymbol{w}} = (\hat{w}_1, \hat{w}_2, \ldots, \hat{w}_p)$ and bias $\hat{b}$ and m constraints
- This is a classic but fiddly optimisation problems
- It can be solved in $O(p^3)$ 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 with time complexity $O(m^3)$

Outline

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



Extended Feature Space

- We can generalise the SVM if we map all our features vectors to an extended feature space

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

- The components of $\boldsymbol{\phi}(\boldsymbol{x})$ will typically be (non-linear) functions of $\boldsymbol{x}$ (e.g. $\phi_1(\boldsymbol{x}) = x_1^2, \phi_2(\boldsymbol{x}) = x_2^2, \phi_3(\boldsymbol{x}) = \sqrt{2}x_1x_2$)
- We are free to choose whatever mappings we like
- There may be many more components of $\boldsymbol{\phi}(\boldsymbol{x})$ than of $\boldsymbol{x}$ making it easier to find a linear separation of the two classes
- But in the extended feature space (involving $\boldsymbol{\phi}(\boldsymbol{x}) = (\phi_1(\boldsymbol{x}), \phi_2(\boldsymbol{x}), \ldots, \phi_r(\boldsymbol{x})))$ the time complexity is $O(r^3)$

Lagrangian

- In the extended feature space we can find a separating plane (given by $\boldsymbol{w}$ and b) with maximum margine by solving the problem

$$\min_{\boldsymbol{w},b} \frac{\|\boldsymbol{w}\|^2}{2} \quad \text{subject to } y_k(\langle \boldsymbol{w}, \boldsymbol{\phi}(\boldsymbol{x}_k)\rangle - b) \geq 1 \text{ for all } k = 1, 2, \ldots, m$$

- We can write this as a Lagrange problem

$$\min_{\boldsymbol{w},b} \max_{\boldsymbol{\alpha} \geq 0} \mathcal{L}(\boldsymbol{w}, b, \boldsymbol{\alpha})$$

where

$$\mathcal{L}(\boldsymbol{w}, b, \boldsymbol{\alpha}) = \frac{\|\boldsymbol{w}\|^2}{2} - \sum_{k=1}^{m} \alpha_k \Big(y_k \left(\langle \boldsymbol{w}, \boldsymbol{\phi}(\boldsymbol{x}_k)\rangle - b \right) - 1 \Big)$$

subject to $\alpha_k \geq 0$

Obtaining the Dual Form of the Problem

- Differentiating the Lagrangian with respect to $\boldsymbol{w}$

$$\mathcal{L}(\boldsymbol{w}, b, \boldsymbol{\alpha}) = \frac{1}{2}\|\boldsymbol{w}\|^2 - \sum_{k=1}^{m} \alpha_k \Big(y_k \left(\langle \boldsymbol{w}, \boldsymbol{\phi}(\boldsymbol{x}_k)\rangle - b \right) - 1 \Big)$$

- $\boldsymbol{\nabla}_{\boldsymbol{w}} \mathcal{L} = \boldsymbol{w} - \sum_{k=1}^{m} \alpha_k y_k \boldsymbol{\phi}(\boldsymbol{x}_k) = 0$ implies that $\boldsymbol{w}^* = \sum_{k=1}^{m} \alpha_k y_k \boldsymbol{\phi}(\boldsymbol{x}_k)$
- $\frac{\partial \mathcal{L}}{\partial b} = \sum_{k=1}^{m} \alpha_k y_k = 0$ implies $\sum_{k=1}^{m} \alpha_k y_k = 0$
- Substituting back into the Lagrangian

$$\max_{\boldsymbol{\alpha} \geq \boldsymbol{0}} \sum_{k=1}^{m} \alpha_k - \frac{1}{2} \sum_{k,l=1}^{m} \alpha_k \alpha_l y_k y_l \langle \boldsymbol{\phi}(\boldsymbol{x}_k), \boldsymbol{\phi}(\boldsymbol{x}_l)\rangle$$

The Dual Problem

- The dual problem is now to find α_k's that maximise

$$\mathcal{L}(\boldsymbol{\alpha}) = \sum_{k=1}^{m} \alpha_k - \frac{1}{2} \sum_{k,l=1}^{m} \alpha_k \alpha_l y_k y_l \langle \boldsymbol{\phi}(\boldsymbol{x}_k), \boldsymbol{\phi}(\boldsymbol{x}_l)\rangle$$

- subject to constraints

$$\sum_{k=1}^{m} \alpha_k y_k = 0 \qquad \forall k = 1, 2, \ldots, m \quad \alpha_k \geq 0$$

- The Hessian of $\mathcal{L}(\boldsymbol{\alpha})$ has elements $H_{kl} = -y_k y_l \langle \boldsymbol{\phi}(\boldsymbol{x}_k), \boldsymbol{\phi}(\boldsymbol{x}_l)\rangle$ so $\boldsymbol{v}^{\mathsf{T}}\mathbf{H}\boldsymbol{v} = -\|\sum_k v_k y_k \phi_k(\boldsymbol{x}_k)\|^2 \leq 0$ (note this is negative semi-definite so there is a unique maximum)

Kernel Trick

- We will show in the next lecture that if $K(\boldsymbol{x}, \boldsymbol{y})$ is a positive semi-definite function then it can always be written as

$$K(\boldsymbol{x}, \boldsymbol{y}) = \langle \boldsymbol{\phi}(\boldsymbol{x}), \boldsymbol{\phi}(\boldsymbol{y})\rangle$$

- As $\langle \boldsymbol{\phi}(\boldsymbol{x}_k), \boldsymbol{\phi}(\boldsymbol{x}_l)\rangle$ appears in the dual problem we can express the dual problem as finding α_k's that maximise

$$\mathcal{L}(\boldsymbol{\alpha}) = \sum_{k=1}^{m} \alpha_k - \frac{1}{2} \sum_{k,l=1}^{m} \alpha_k \alpha_l y_k y_l K(\boldsymbol{x}_k, \boldsymbol{x}_l)$$

- We therefore never have to compute $\boldsymbol{\phi}(\boldsymbol{x})$

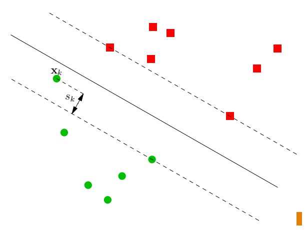
Sequential Minimal Optimisation

- One of the most efficient techniques for training SVMs is *Sequential Minimal Optimisation* or SMO
- This takes two Lagrange multipliers α_i and α_j and adjusts them to maximise the dual objective function
- This is very quick as it can be done in closed form
- Note that because $\sum_{k=1}^{m} y_k \alpha_k = 0$ we have to change at least two variables at the same time
- A heuristic is used to choose good pairs of α's to optimise
- Run until close to the optimum

Soft Margins

- We can relax the margin constraints by introducing *slack variables*, $s_k \geq 0$

$$y_k(\langle \boldsymbol{x}_k, \boldsymbol{w}\rangle - b) \geq 1 - s_k$$



- Minimise $\frac{\|\boldsymbol{w}\|^2}{2} + C\sum_{k=1}^{n} s_k$
- Larger C punishes slack variables more

Dual Problem with Slack Variables

- The Lagrangian with slack variables is

$$\mathcal{L} = \frac{1}{2}\|\boldsymbol{w}\|^2 + C\sum_{k=1}^{m} s_k - \sum_{k=1}^{m} \alpha_k \Big(y_k \left(\langle \boldsymbol{w}, \boldsymbol{\phi}(\boldsymbol{x}_k) \rangle - b \right) - 1 + s_k \Big) - \sum_{k=1}^{m} \beta_k s_k$$

  where β_k are Lagrange multipliers that ensure $s_k \geq 0$ (note that $\beta_k \geq 0$—this is the KKT condition)

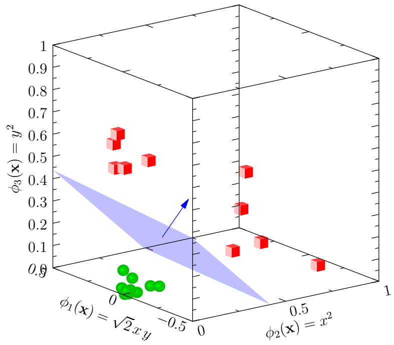
- Now minimising with respect to s_i

$$\frac{\partial \mathcal{L}}{\partial s_i} = C - \alpha_i - \beta_i = 0$$

- Or $\alpha_i = C - \beta_i$. Since $\beta_i \geq 0$ the constraint is $\alpha_i \leq C$ (recall also $\alpha_i \geq 0$)

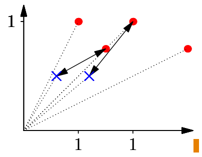
Outline

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



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)

Optimising C

- Recall that we can introduce soft-margins using slack variables where we minimise $\frac{\|\hat{\boldsymbol{w}}\|^2}{2} + C\sum_{k=1}^{m} s_k$ subject to constraints
- 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})
- Measure performance on a validation set

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
- Kernels 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}

Multi-Class Problems

- By construction SVMs separate only two classes
- If we have a multi-class problem we have to use multiple SVMs
- There are two major ways practitioners do this

  One-versus-all: for each class, train a separate classify to determine that class versus all others
  All-pairs: train a classify for all pairs of classes

- In both cases choose the class which the classifier is most certain about
- Beware SVMs don't like imbalanced datasets

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, (now old), scikit-learn, etc.
- These will often automate normalisation of data and grid search for parameters

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
- The **dual problem** of an SVM is particularly simple, especially if we use a positive semi-definite kernel (we explore these in the next lecture)