Lecture 13. Introduction to Support Vector Machines

COMP90051 Statistical Machine Learning

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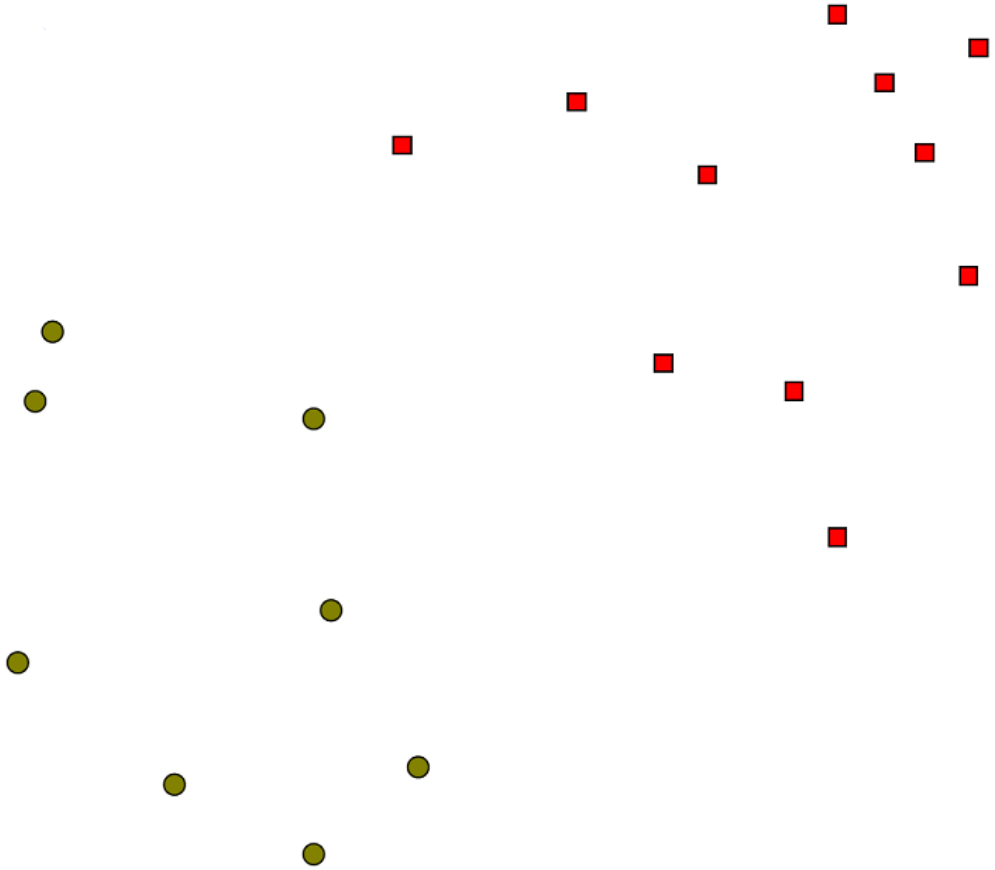
Content is based on slides provided by Ben Rubinstein

Linear Support Vector Machines (SVM)

Yet another linear model that can be regularised

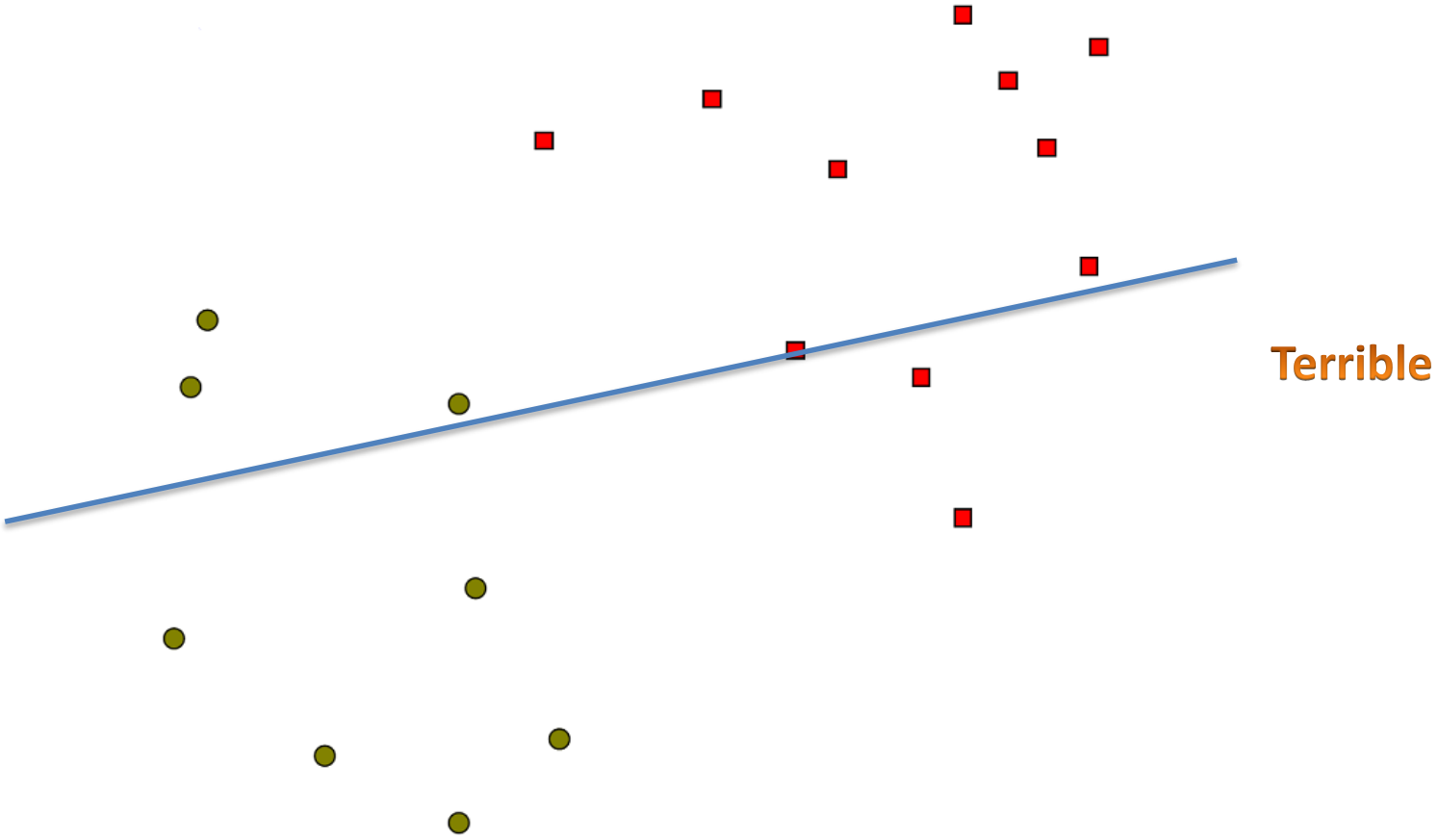
Support Vector Machines: Intuition

- What linear classifier to choose?



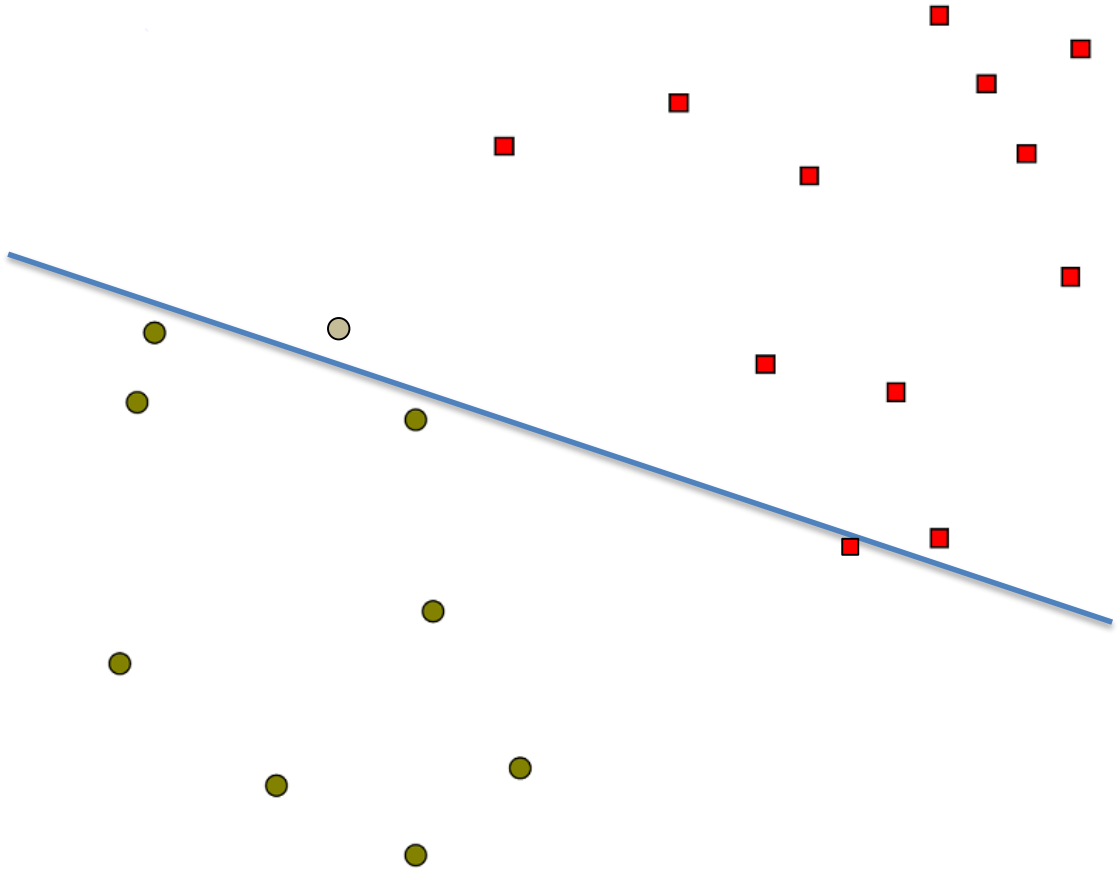
Support Vector Machines: Intuition

- What linear classifier to choose?



Support Vector Machines: Intuition

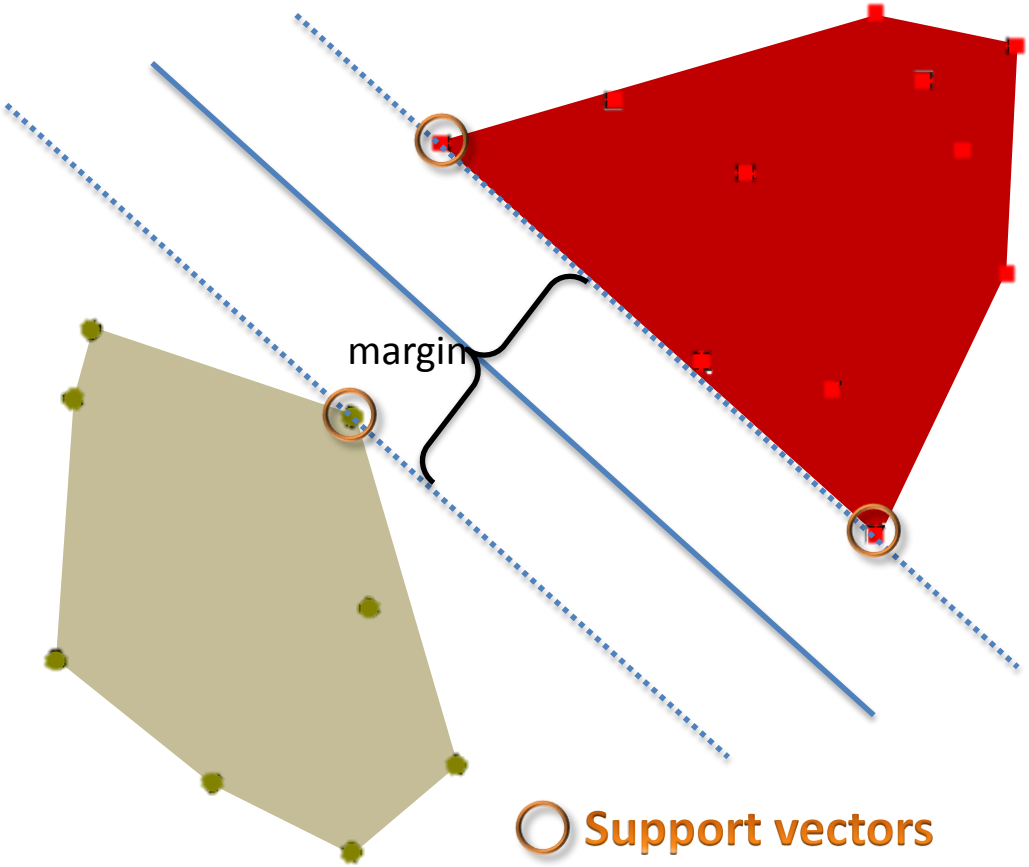
- What linear classifier to choose?



Good train error
Bad test error

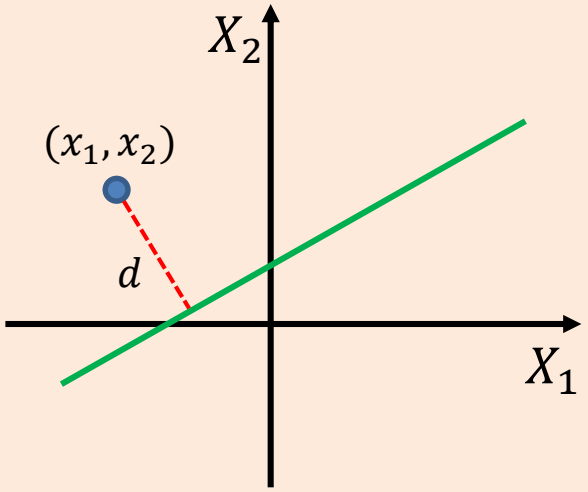
Support Vector Machines: Intuition

- What linear classifier to choose?



(very brief) Revision of geometry

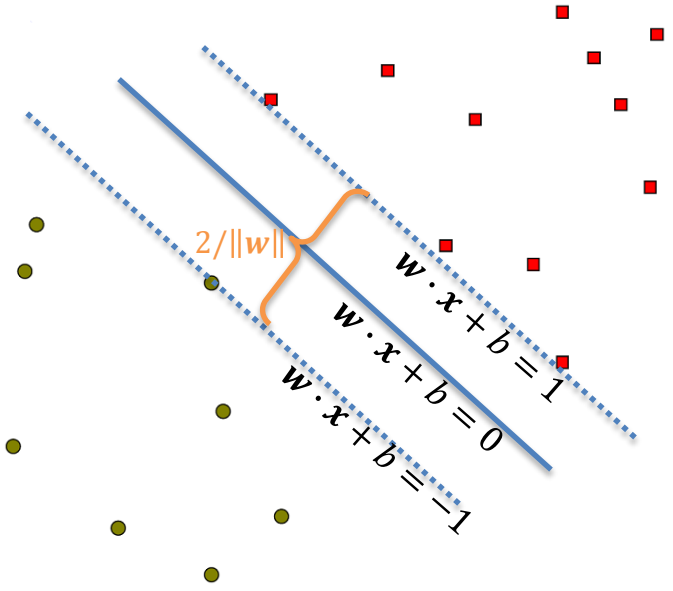
- Line = set of points (x_1, x_2) that satisfy $w_1 x_1 + w_2 x_2 + b = 0$
- Plane ➔ $w_1 x_1 + w_2 x_2 + w_3 x_3 + b = 0$
- Hyperplane ➔ $\sum_{i=1}^{n} w_i x_i + b = 0$



- Note: we can multiply w_i, b by a constant without changing the (hyper-)plane
- Distance from point $\boldsymbol{x}$ to (hyper-)plane is $d = \frac{|\boldsymbol{w}^T \boldsymbol{x} + b|}{\|\boldsymbol{w}\|}$
- We can rescale so that $\boldsymbol{w}^T \boldsymbol{x} + b = 1$, and get $d = \frac{1}{\|\boldsymbol{w}\|}$

Linear SVM parameters

- Goal: max margin hyperplane
- Hyperplane parameters
  - Normal vector $\boldsymbol{w}$
  - Offset b
- Scale parameters so that
  - Negative data: $\boldsymbol{w} \cdot \boldsymbol{x} + b \leq -1$
  - Positive data: $\boldsymbol{w} \cdot \boldsymbol{x} + b \geq +1$
- Then margin is $2/\|\boldsymbol{w}\|$



Linear SVM algorithm

- If linearly separable data: the optimal classifier is

$$\min_{\boldsymbol{w},b} \ \frac{1}{2}\|\boldsymbol{w}\|^2$$

subject to $y_i(\boldsymbol{w}\cdot\boldsymbol{x}_i + b) \geq 1, \ \forall i$

Hard-margin SVM

- In general, relax to allow training errors
  - Intuitively minimise: $\frac{1}{2}\|\boldsymbol{w}\|^2 + C \cdot average\big(loss(y_i, \hat{y}_i)\big)$
  - Formally, introduce "slacks" $\xi_i \geq 0$'s

$$\min_{\boldsymbol{w},b,\boldsymbol{\xi}} \left(\frac{1}{2}\|\boldsymbol{w}\|^2 + \frac{C}{n}\sum_{i=1}^{n} l(\xi_i)\right)$$

subject to $y_i(\boldsymbol{w}\cdot\boldsymbol{x}_i + b) \geq 1 - \xi_i, \ \forall i$

Soft-margin SVM

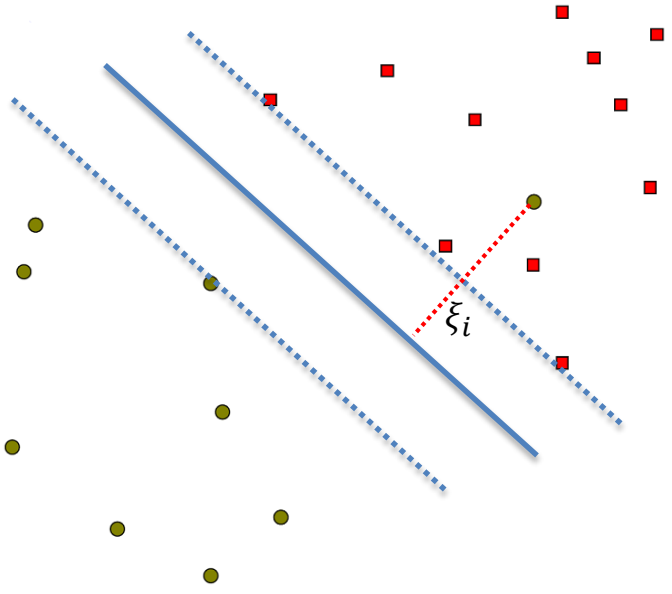
Soft-margin SVM

"Slack" variables: it is OK for some points to be on the wrong side

Still, closer they are to the margin the better

$$\min_{\boldsymbol{w},b,\boldsymbol{\xi}} \left(\frac{1}{2}\|\boldsymbol{w}\|^2 + \frac{C}{n}\sum_{i=1}^{n} l(\xi_i) \right)$$

subject to $y_i(\boldsymbol{w}\cdot\boldsymbol{x}_i + b) \geq 1 - \xi_i, \ \forall i$



Déjà vu?

Soft-margin SVM: $\min_{\mathbf{w}} \left(\frac{1}{2}\|\boldsymbol{w}\|^2 + C \cdot average\big(loss(y_i, \hat{y}_i)\big) \right)$

model class complexity

training error

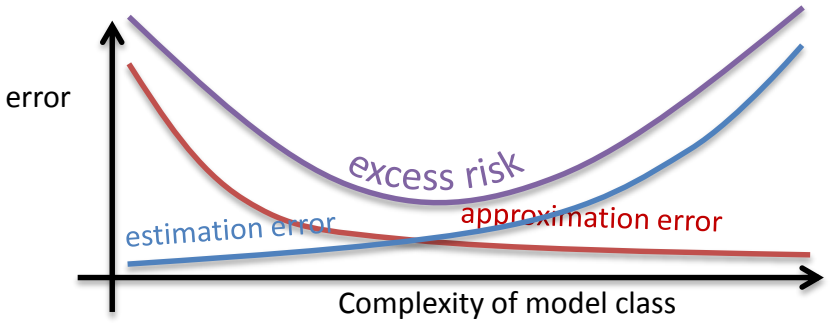
Ridge regression: $\min_{\boldsymbol{w}} \left(\lambda\|\boldsymbol{w}\|^2 + \sum_i (y_i - \boldsymbol{X}_i.\boldsymbol{w})^2 \right)$

model class complexity

training error

Soft-margin parameter *C*

- Varies effective complexity
- Theory: should grow like $O(\sqrt{n})$
- Practice: set with cross-validation



Training the SVM

- Loss function
  - Must be convex to make minimisation tractable
  - Typically: linear (hinge), squared
- Solving the minimisation
  - Convex → unique global optimum guaranteed
  - Could use gradient descent, but there are better ways
  - Constrained Quadratic Program → standard
  - Many tricks to improve speed or memory (chunking, SMO)
- Non-linear SVM coming up (“kernelisation”)

SVM summary (so far)

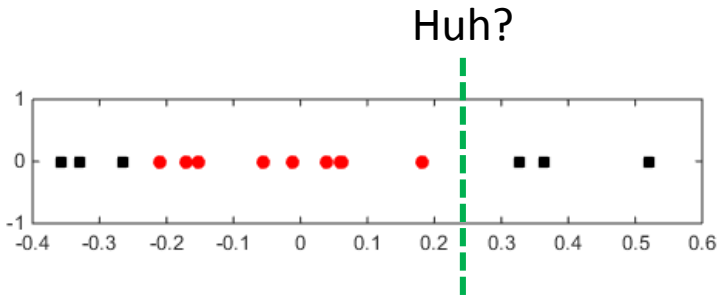
Non-parametric	There are essentially parameters per support vector (next time)
Discriminative	SVM models P(Y|X) – the decision boundary – nothing about P(X)
Regularised, frequentist	Extent of regularisation controlled by varying the soft-margin parameter; Justification is via theoretical bounds on risk
Computational efficiency	Mediocre cubic polynomial in #data, or #features, for training
Accuracy (aka statistical efficiency)	Typically very good empirically; Exists nice theory on error bounds; Much better if non-linear in some cases.
Packages	http://svmlight.joachims.org http://www.csie.ntu.edu.tw/~cjlin/libsvm Pyhton, R packages, MatLab, Weka (Java), etc.

The Kernel Trick

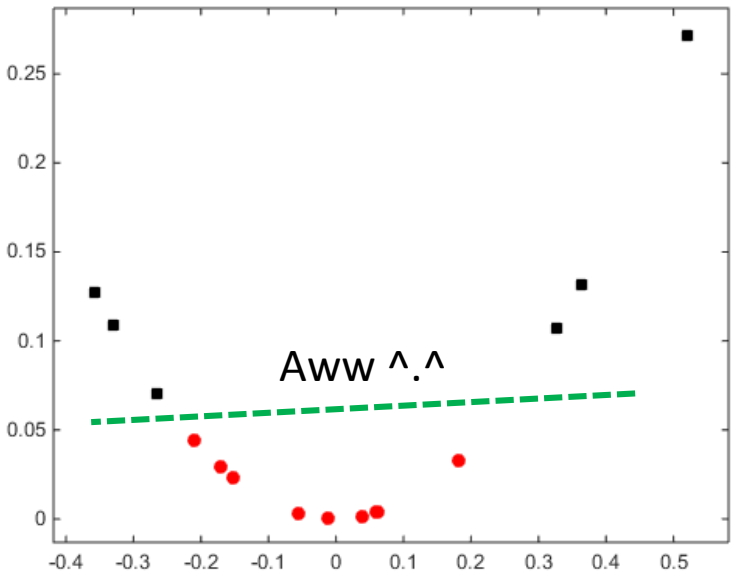
Very powerful method that enables effective use of linear methods for non-linear data

Feature space mapping: example 1

- Consider a binary classification problem
- Each example has one feature $[x_1]$
- Not linearly separable

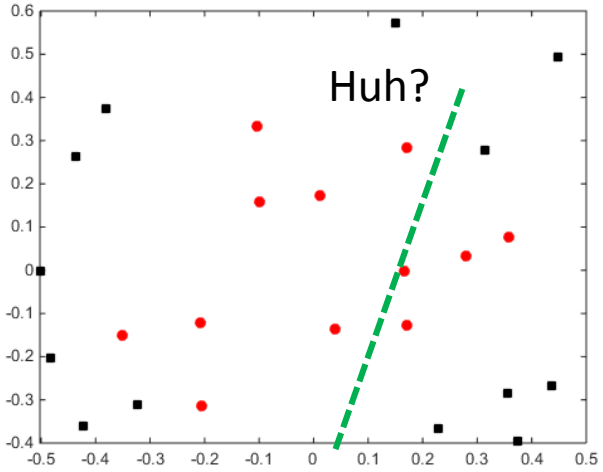


- Now 'add' a feature $x_2 = x_1^2$
- Each point is now $[x_1, x_1^2]$
- Linearly separable!

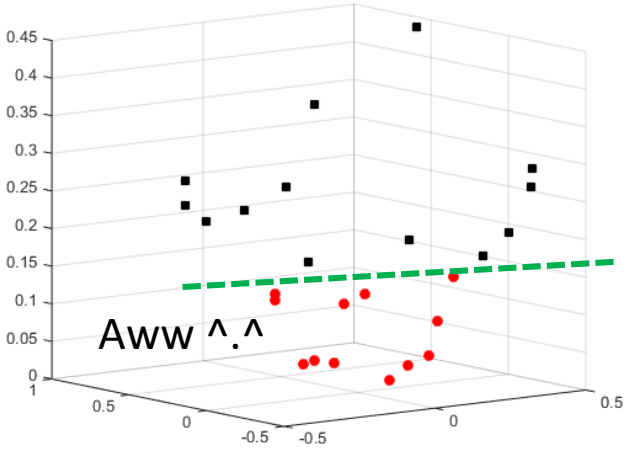


Feature space mapping: example 2

- Consider a binary classification problem
- Each example has features $[x_1, x_2]$
- Not linearly separable



- Now 'add' a feature $x_3 = x^2 + x_2^2$
- Each point is now $[x_1, x_2, x_1^2 + x_2^2]$
- Linearly separable!



Observation 1

- A non-linear boundary in original feature space can become a linear boundary in a transformed space
- Denote this transformation as $\varphi(\boldsymbol{x})$
- For example, $\varphi([x_1, x_2]) = [x_1, x_2, x_1^2 + x_2^2]$
- Note $\varphi(\boldsymbol{x})$ has more dimensions than $\boldsymbol{x}$
  - Commonly used $\varphi(\boldsymbol{x})$ often have very large dimensionality
  - Sometimes $\varphi(\boldsymbol{x})$ have infinite dimensionality!

Naïve workflow

- Choose/design a linear model
- Choose/design a transformation $\varphi(\boldsymbol{x})$
- For each training example, and for each new instance compute $\varphi(\boldsymbol{x})$
- Train classifier/Do predictions

- Problem: impractical/impossible to compute $\varphi(\boldsymbol{x})$ for high/infinite-dimensional $\varphi(\boldsymbol{x})$

Observation 2

- For a large class of linear models, both parameter estimation and computing predictions depend on data only in a form of dot product
- Dot product $\boldsymbol{xy} = \sum_{i=1}^{d} x_i y_i$
- In transformed space $\varphi(\boldsymbol{x})\varphi(\boldsymbol{y}) = \sum_{i=1}^{d'} \varphi(\boldsymbol{x})_i \varphi(\boldsymbol{y})_i$
- Kernel is a function that can be expressed as a dot product in some feature space $K(\boldsymbol{x}, \boldsymbol{y}) = \varphi(\boldsymbol{x})\varphi(\boldsymbol{y})$

Kernel trick: example

- For many transformations there is a shortcut computation of the dot product!
- For example, consider two points in original space $\boldsymbol{x} = [x_1]$ and $\boldsymbol{y} = [y_1]$
- Consider transformation $\varphi(\boldsymbol{x}) = [x_1^2, \sqrt{2c}x_1, c]$
- Then $\varphi(\boldsymbol{x})\varphi(\boldsymbol{y}) = (x_1^2 y_1^2 + 2cx_1 y_1 + c^2)$
- This simplifies to $\varphi(\boldsymbol{x})\varphi(\boldsymbol{y}) = (x_1 y_1 + c)^2$
- Here $K(\boldsymbol{x}, \boldsymbol{y}) = (x_1 y_1 + c)^2$ is called kernel

Kernel trick

- For a pair of data points in original space kernel $K(\boldsymbol{x}, \boldsymbol{y})$ can be used to compute dot product in the transformed space
- Computing the transformation $\varphi(\boldsymbol{x})$ as such is not necessary!
- Kernel can be computed in $O(d)$, whereas computing $\varphi(\boldsymbol{x})$ requires $O(d')$, where $d' \gg d$ or $d' = \infty$

Summary

- Linear SVM aims to maximise a separating margin
- Soft-margin SVM allows some instances to be misclassified
- Soft-margin SVM includes regularisation parameter

- When data is not linearly separable, transforming the feature space can make it linearly separable
- Many linear methods only require data in form of dot products
- Kernel trick – fast computation of dot products in very high dimensional feature spaces