SUPPORT VECTOR MACHINES

Applied Analytics: Frameworks and Methods 1

Outline

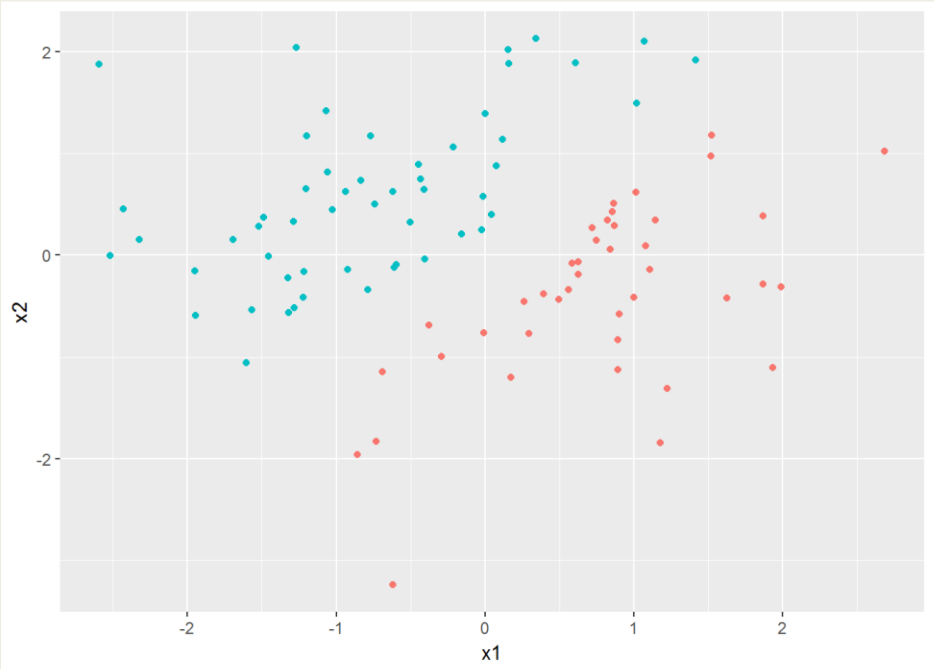
- Intuition behind support vector machines
- Linear classifiers
- Feature expansion to accommodate non-linear decision boundaries
- Polynomial and Radial Basis Function kernels
- SVM vs. logistic regression
- Implementation of SVM in R

Support Vector Machines

- Constructs a hyperplane or set of hyperplanes in a high dimensional space which can be use for both classification and regression.
- It is *not that* statistical!
- Flexible and powerful method for making predictions but models are not easy to interpret.

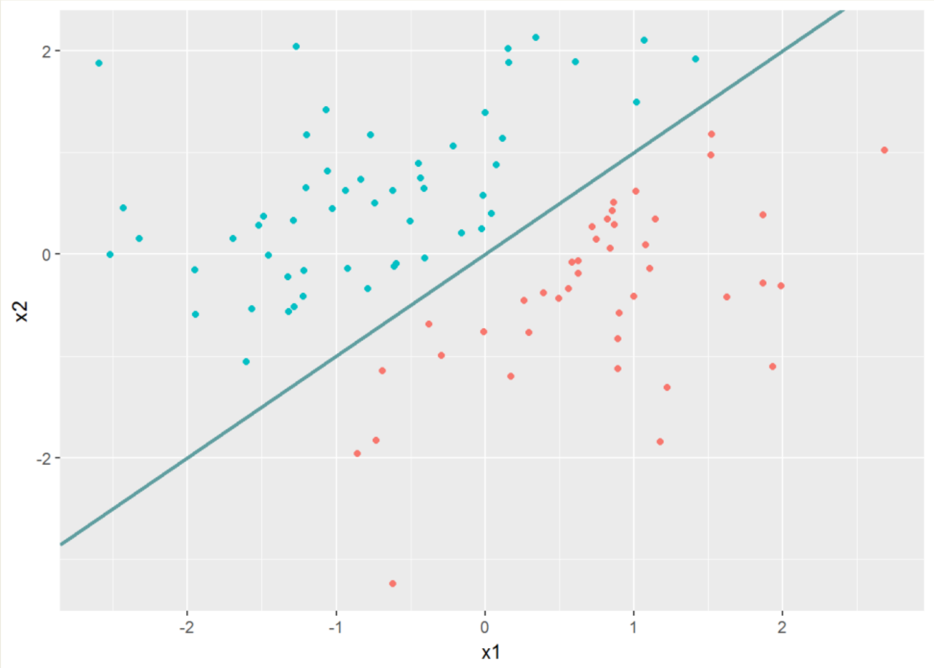
The Intuition

- Begins with trying to find a plane that separates classes in feature space
- Which is great if the classes are linearly separable as seen in the figure.



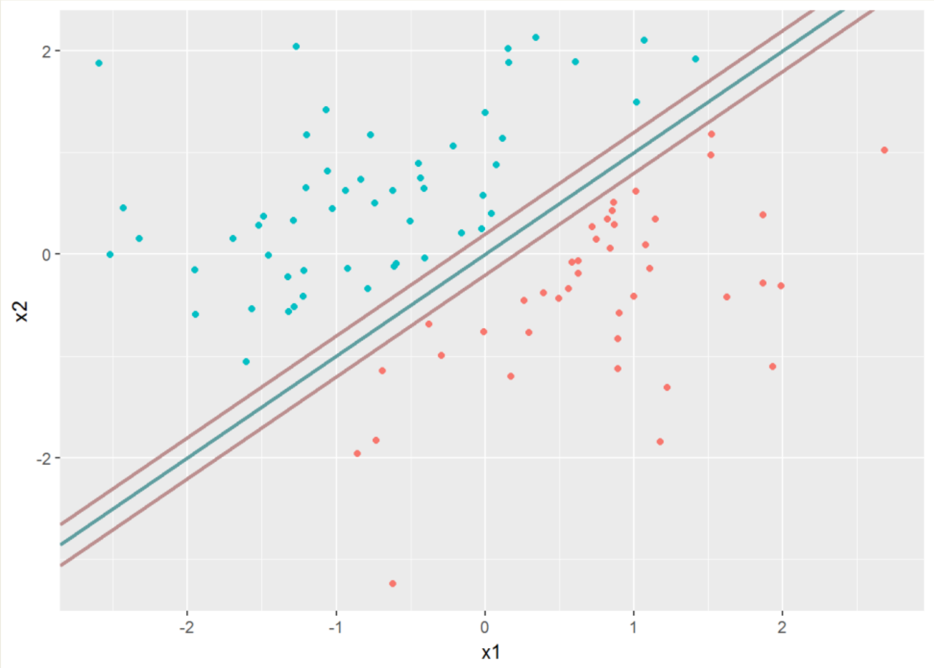
The Intuition

- Fitting a Classifier or Hyperplane to linearly separable classes
- But, these classes can be separated by a very large number of hyperplanes



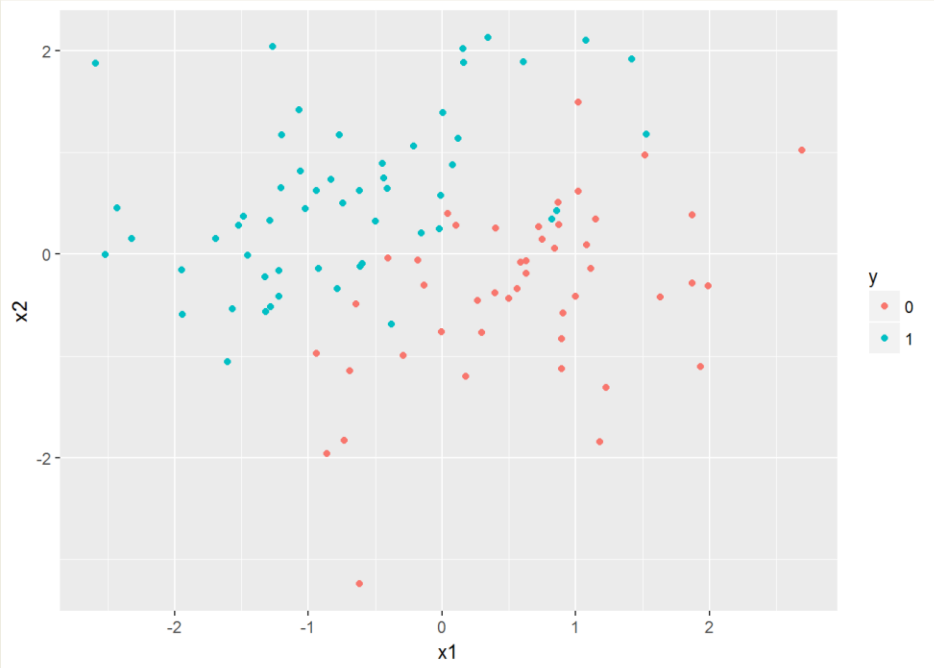
The Intuition

- The decision boundary chosen is the one that has the biggest margin and is accordingly called Maximum Margin Classifier.



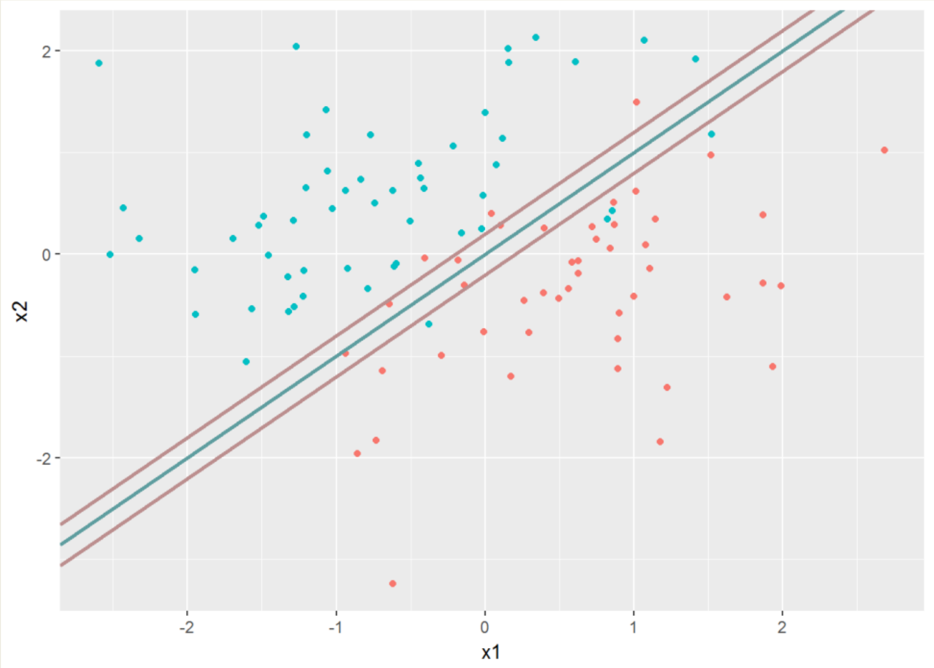
The Intuition

- In practice, classes are seldom linearly separable



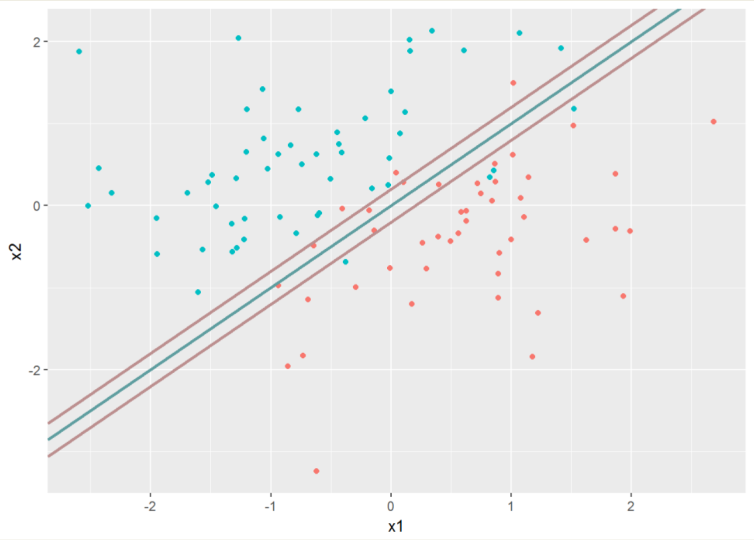
The Intuition

- Therefore, the requirement of a hard margin is relaxed in favor of a soft margin
- The soft margin used is determined by a cost parameter
- Higher cost – narrower margins

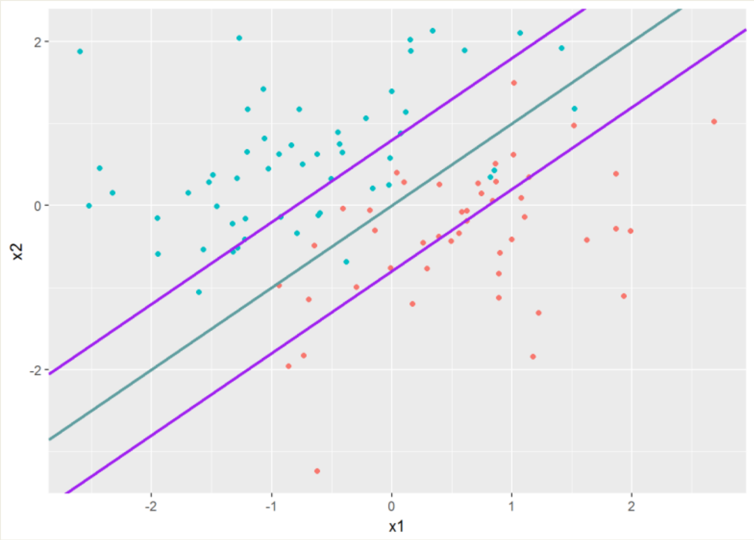


The Intuition

High Cost



Low Cost



Support Vector Machines

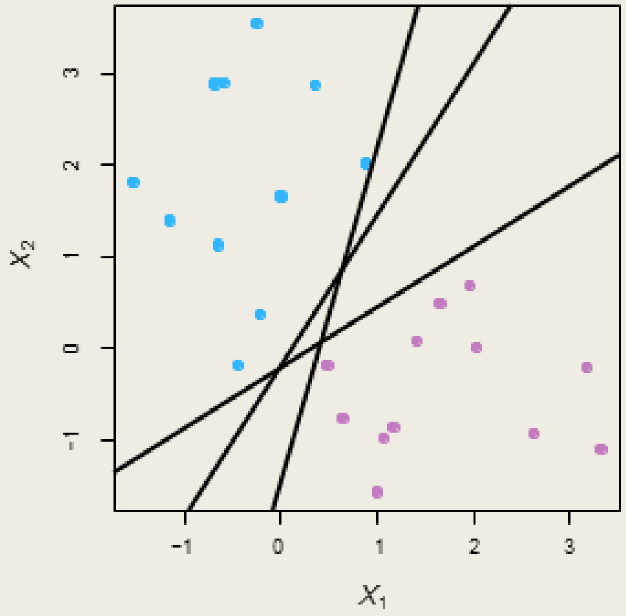
- Begins with trying to find a plane that separates classes in feature space
- Since, in practice this is difficult, the technique
  - *Looks for a soft margin boundary that separates classes*
  - *Enriches and enlarges the features space to make separation possible*

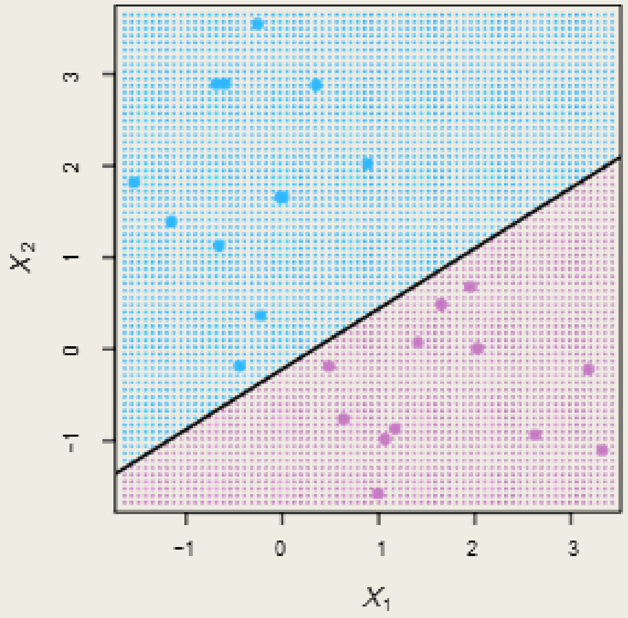
What is a Hyperplane?

- A hyperplane in p dimensions is a flat affine subspace of dimension $p - 1$.
- In general the equation for a hyperplane has the form
- $\beta_0 + \beta_1 X_1 + \beta_2 X_2 + \ldots + \beta_p X_p = 0$
- In $p = 2$ dimensions a hyperplane is a line
- If $\beta_0 = 0$, the hyperplane goes through the origin, otherwise not.
- The vector $\beta = (\beta_1, \beta_2, \cdots, \beta_p)$ is called the normal vector — it points in a direction orthogonal to the surface of a hyperplane

Separating Hyperplanes

- If $f(X) = \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p$, then $f(X) > 0$ for points on one side of the hyperplane, and $f(X) < 0$ for points on the other
- If we code the colored points as $Y_i = +1$ for blue, say, and $Y_i = -1$ for mauve, then if $Y_i \cdot f(X_i) > 0$ for all i, $f(X) = 0$ defines a *separating hyperplane*

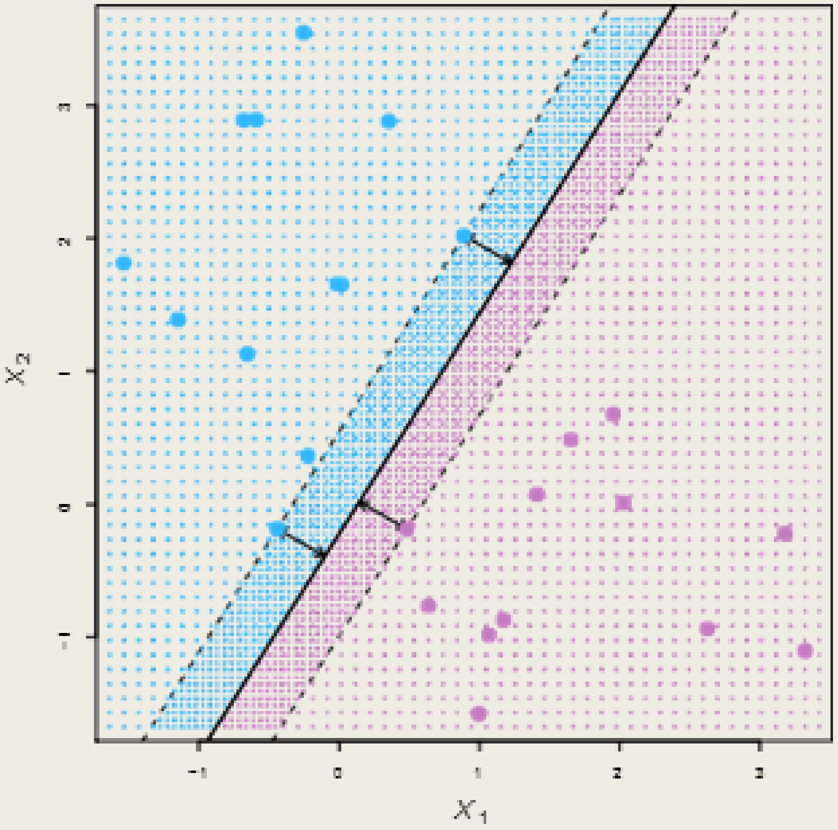




Source: James et al (2017)

Maximum Margin Classifier

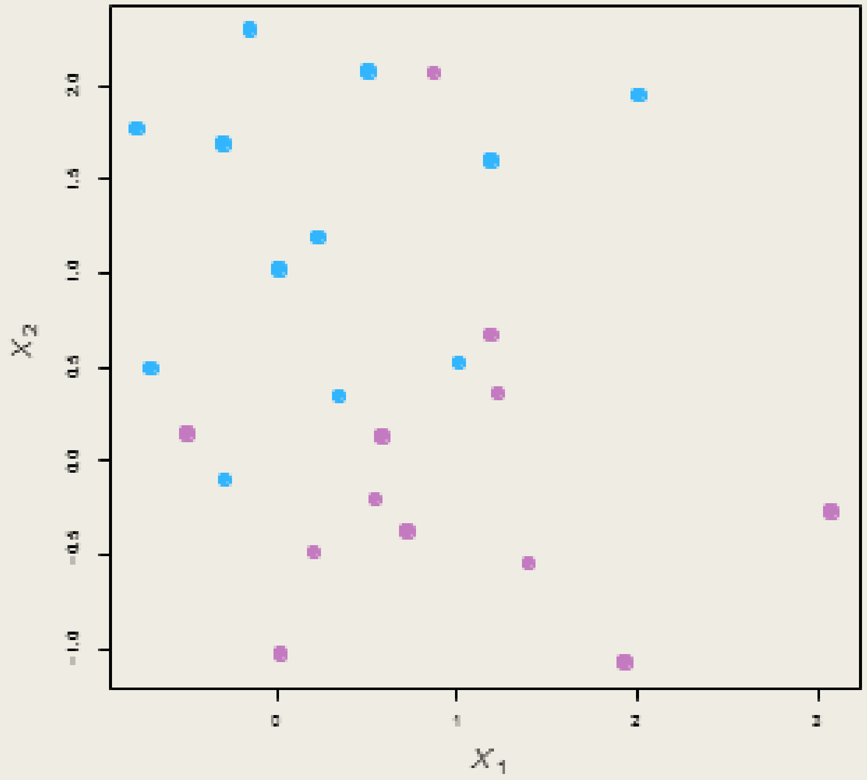
- Among all separating hyperplanes, find the one that makes the biggest gap or margin between the two classes



Source: James et al (2017)

Non-separable Data

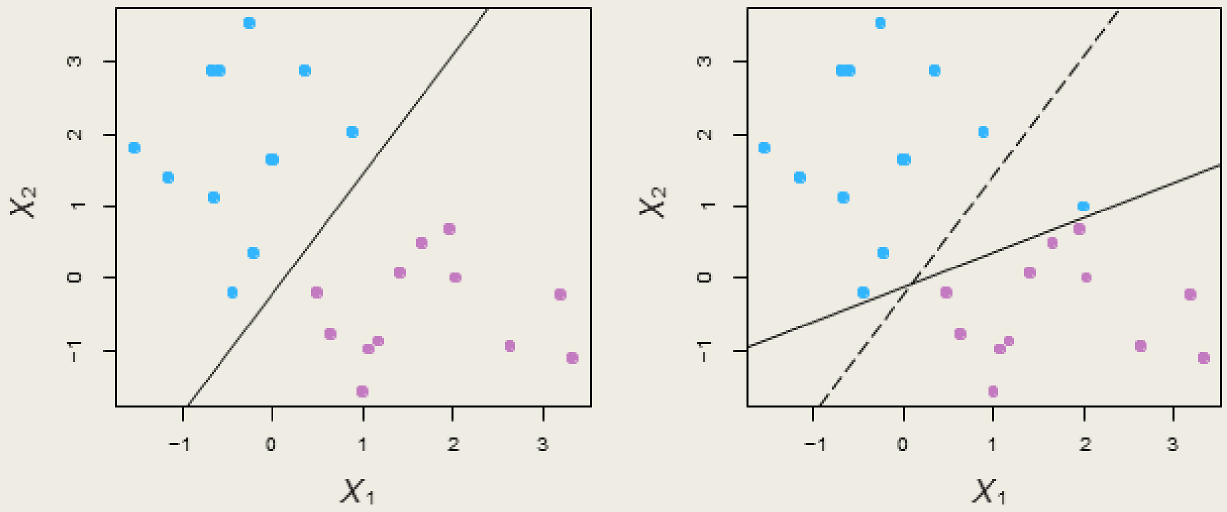
- But, most data is not linearly separable
  - *Exception being when n < p*



Source: James et al (2017)

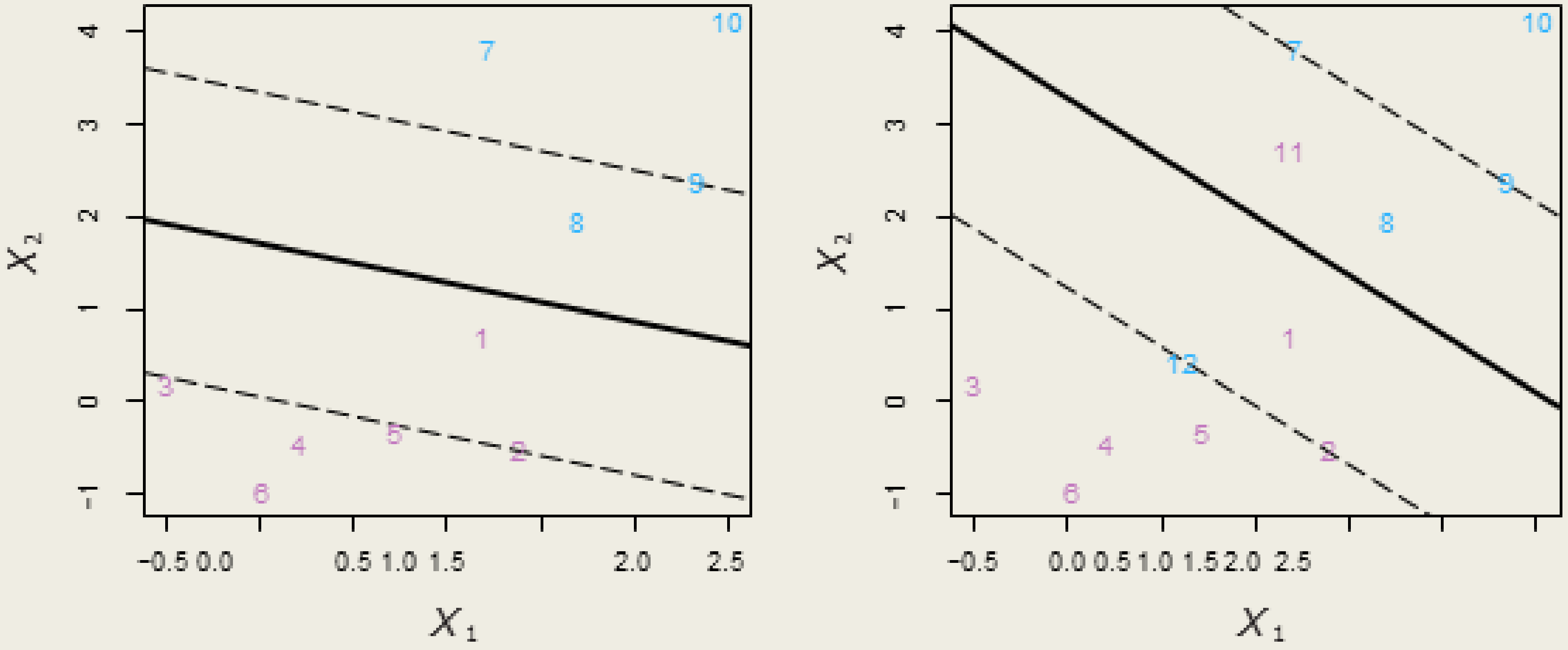
Noisy Data

- Noisy data can lead to a poor solution for the maximal-margin classifier.
- The support vector classifier maximizes a soft margin.



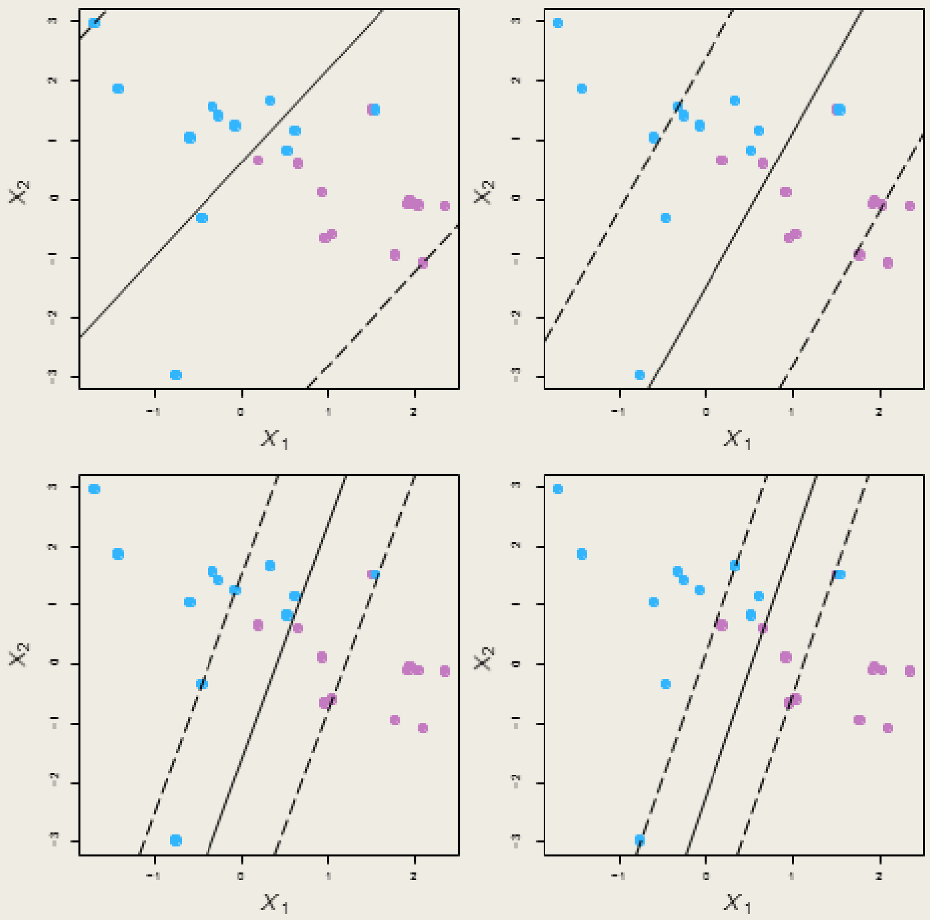
Source: James et al (2017)

Support Vector Classifier



Source: James et al (2017)

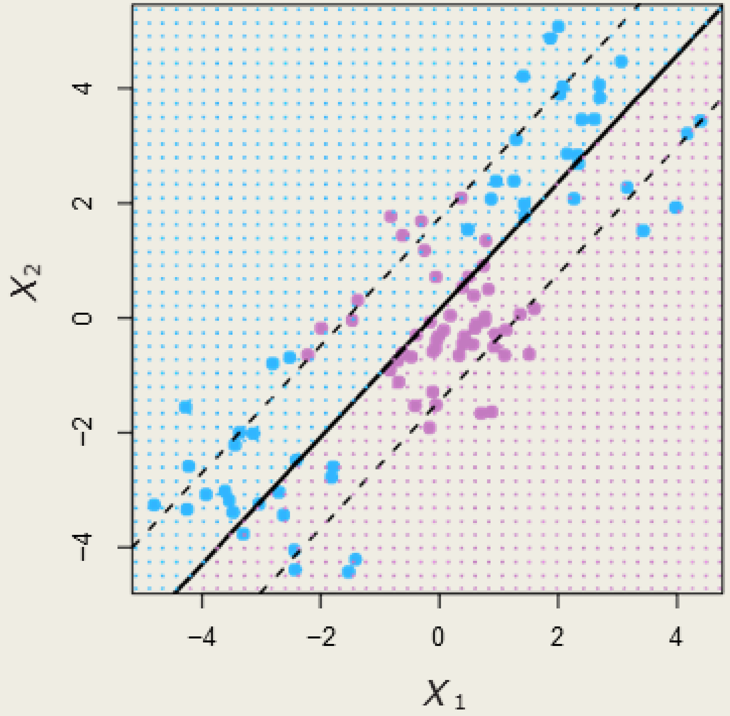
Cost, c, is a Regularization Parameter



Source: James et al (2017)

But, Linear Boundary can Fail

- Sometimes a linear boundary fails, no matter how high the value of C.
- Here is an example.



Source: James et al (2017)

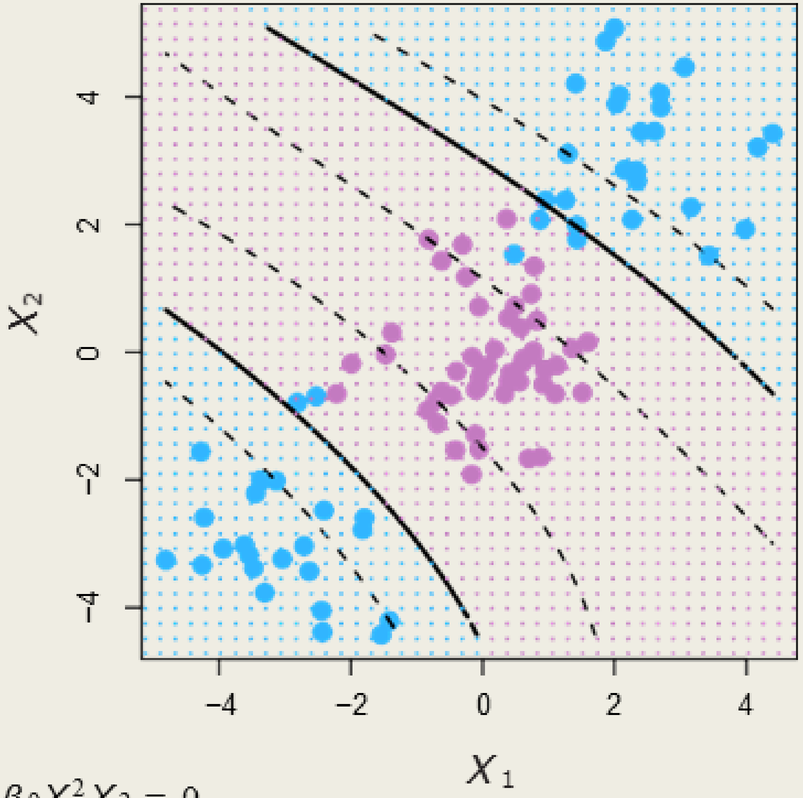
Feature Expansion

- Enlarge the space of features by including transformations, e.g., X_1^2, X_1^3, $X_1X_2^2$. By doing so, we go from a p-dimensional space to an M>p dimensional space.
- Fit a support-vector classifier in the enlarged space
- This results in non-linear decision boundaries in the original space
- E.g., if we use a vector space of (X_1, X_2, X_1^2, X_2^2, X_1X_2)instead of (X_1, X_2)
- Then the decision boundary would be of the form
  - $\beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_1^2 + \beta_4 X_2^2 + \beta_5 X_1X_2 = 0$
- This leads to nonlinear decision boundaries in the original space (quadratic conic sections).

Source: James et al (2017)

Cubic Polynomials

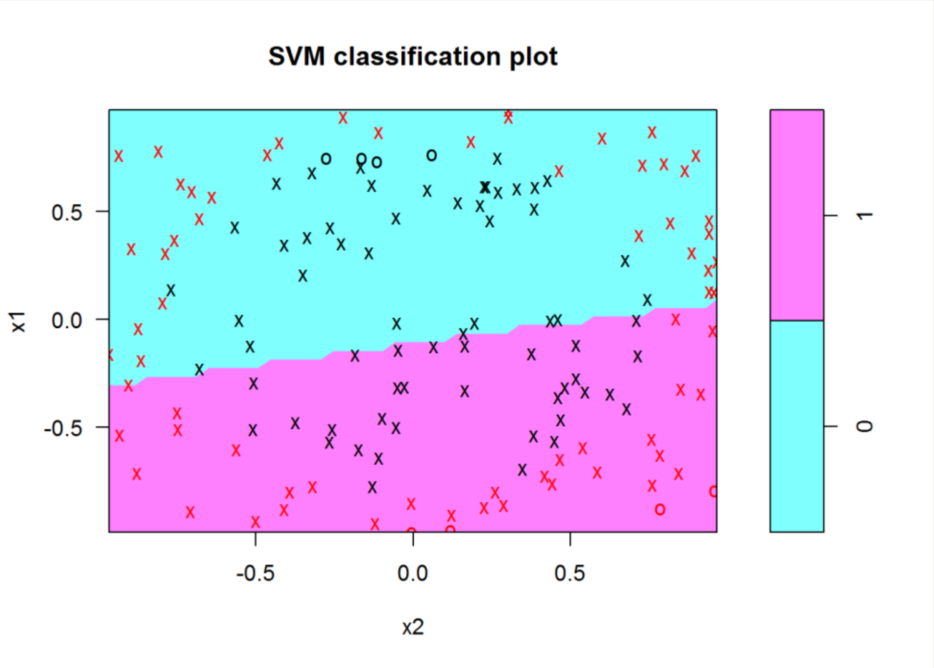
- Basis Expansion of Cubic Polynomials from 2 variables to 9
- The support-vector classifier in the enlarged space solves the problem in the lower-dimensional space

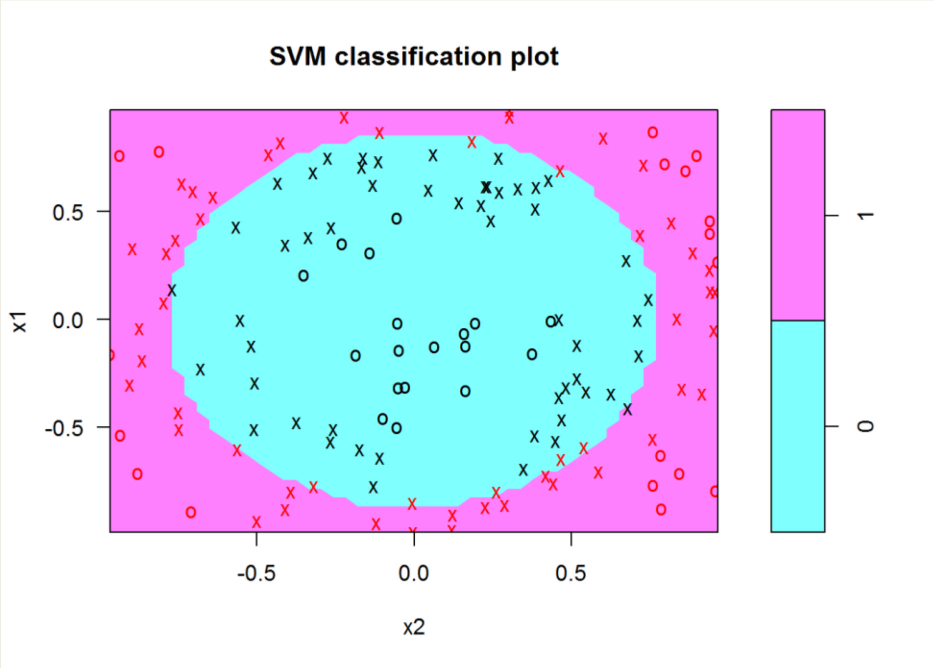


$$\beta_0+\beta_1X_1+\beta_2X_2+\beta_3X_1^2+\beta_4X_2^2+\beta_5X_1X_2+\beta_6X_1^3+\beta_7X_2^3+\beta_8X_1X_2^2+\beta_9X_1^2X_2=0$$

Source: James et al (2017)

Linear vs. Polynomial Kernel



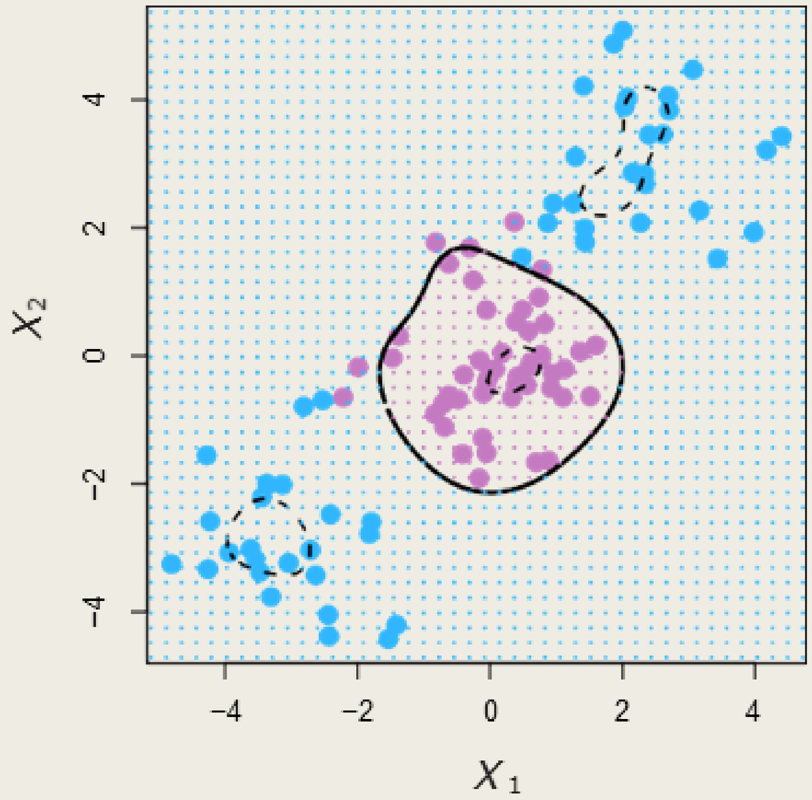


Nonlinearities and Kernels

- Polynomials (especially high-dimensional ones) get wild rather fast.
- There is a more elegant and controlled way to introduce nonlinearities in support-vector classifiers — through the use of kernels.
- If we can compute inner products between observations, we can fit a support vector classifier.
- This is made possible by some simple kernel functions like a Radial Basis Kernel

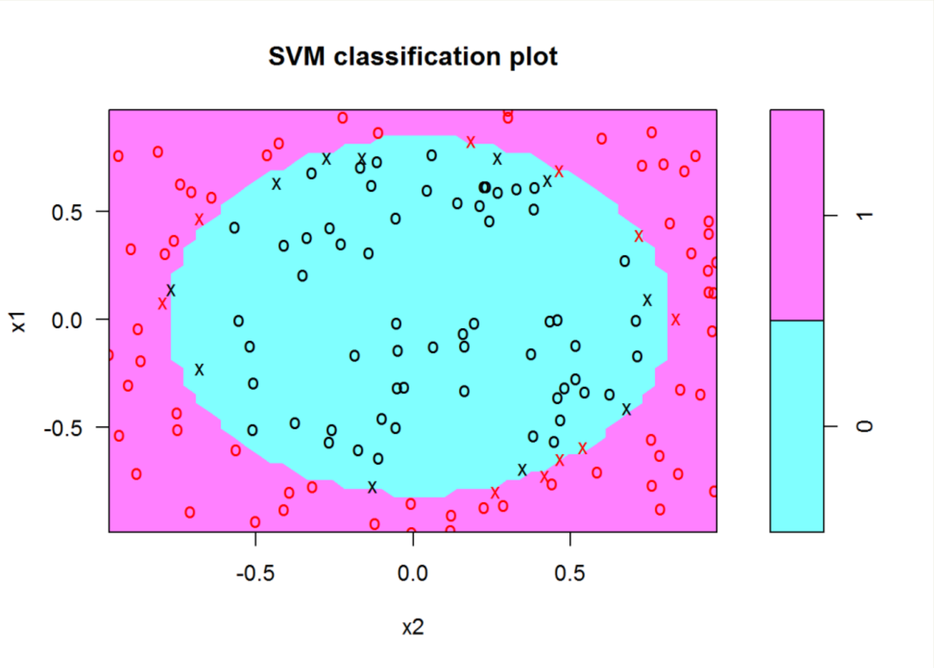
Source: James et al (2017)

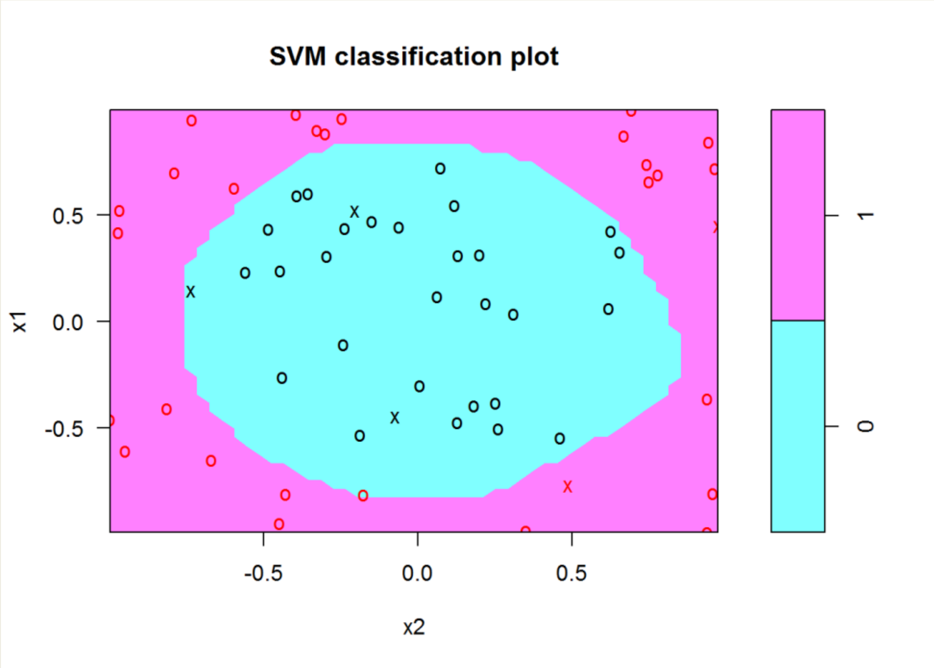
Radial Kernel



Source: James et al (2017)

Polynomial vs. Radial Kernel





SVM for more than 2 classes

- SVM can be extended to a situation with more than two classes. There are two approaches to this
  - *One versus all: Fit k different 2 class SVM classifiers*
  - *One versus One: Fit all pairwise classifiers. Use if k is not too large.*

SVM vs. Logistic Regression

- When classes are (nearly) separable, SVM does better than LR. So does LDA.
- When not, LR (with ridge penalty) and SVM very similar.
- If you wish to estimate probabilities, LR is the choice.
- For nonlinear boundaries, kernel SVMs are popular. Can use kernels with LR and LDA as well, but computations are more expensive.

Illustration

See svm.html

Conclusion

- In this session, we
  - *Examined the intuition behind support vector machines*
  - *Discussed linear classifiers*
  - *Looked at feature expansion to accommodate non-linear decision boundaries*
  - *Examined polynomial and radial kernels*
  - *Compared SVM to logistic regression*
  - *Looked at implementation of SVM in R*