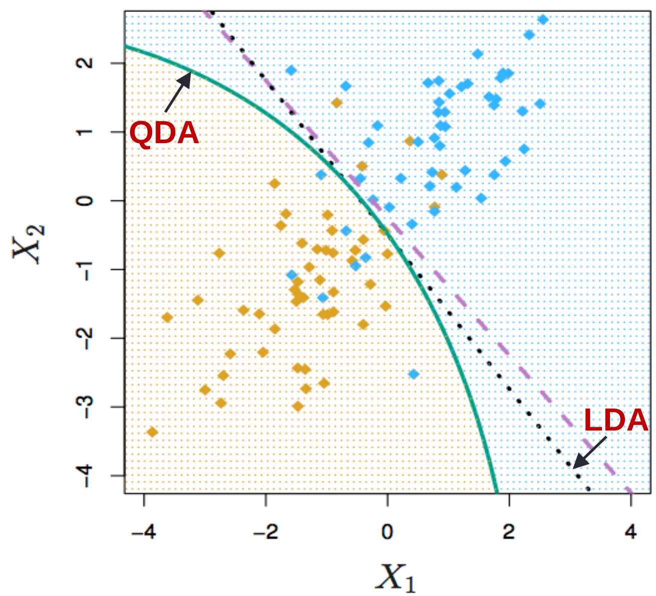
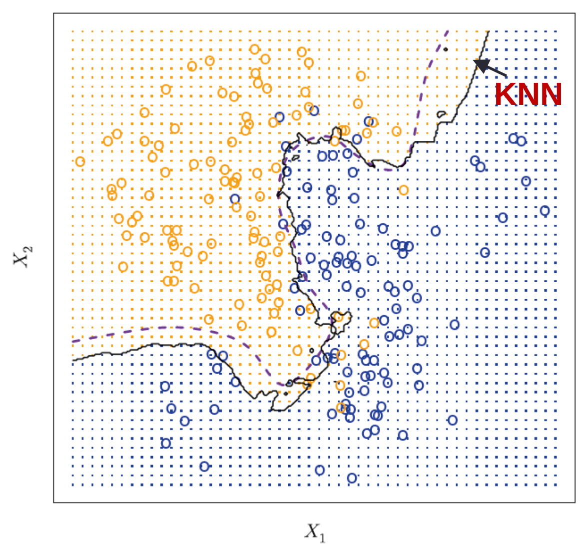
Topic 7. Support Vector Machines

Support Vector Machines (SVM)

- Approach for classification developed in computer science
- One of the best “out of the box” classifiers

- Recall classifiers covered in Chapter 4: logistic regression, LDA, QDA, naïve Bayes, KNN





Outline

- **Maximal Margin Classifier**: classes are separable by a linear boundary

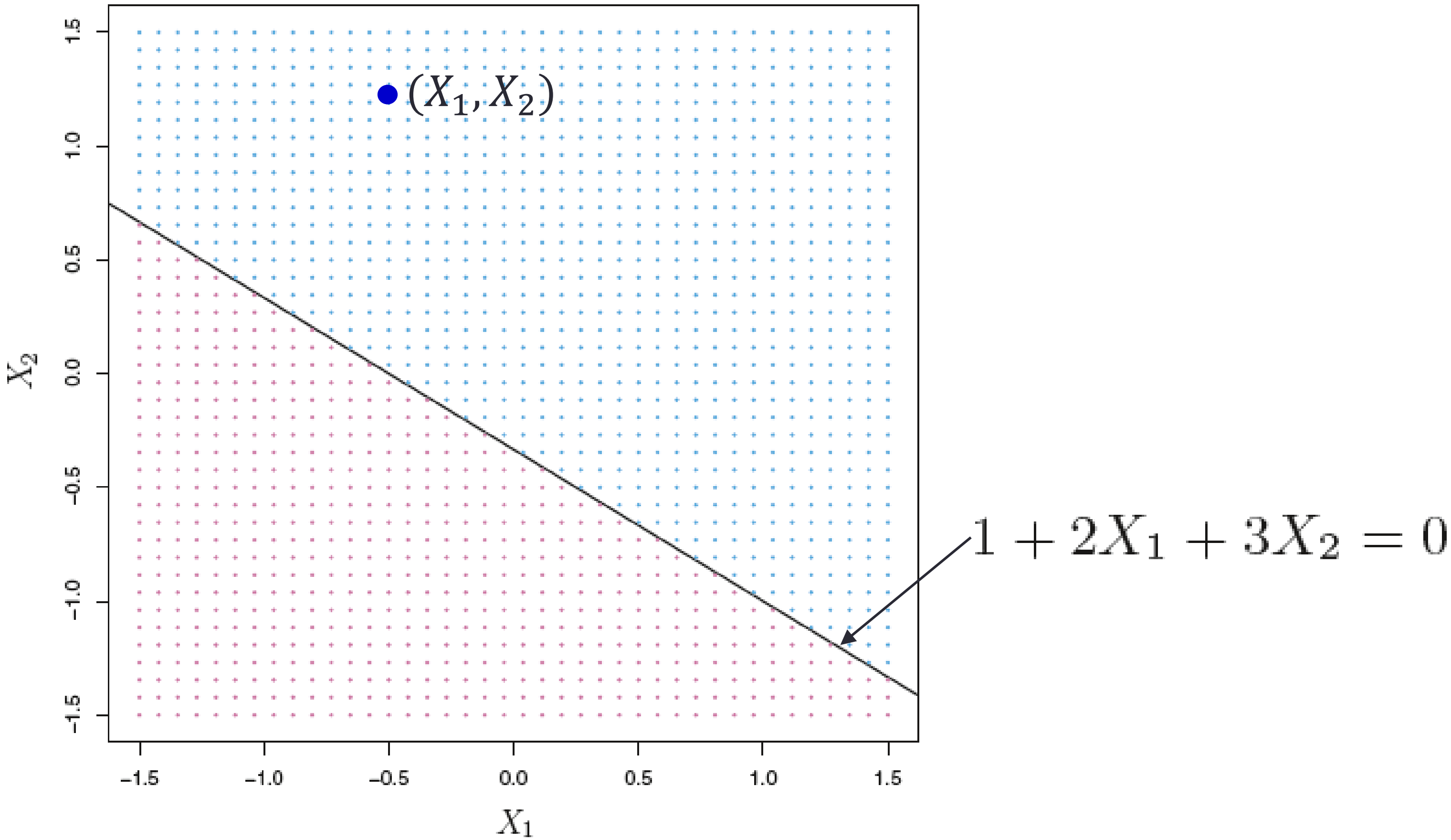
- **Support Vector Classifier**: extend to cases where classes are not separable

- **Support Vector Machine**: extend to non-linear class boundaries

Maximal Margin Classifier

Hyperplane

- In a p-dimensional space, a *hyperplane* is a flat affine subspace of dimension $p - 1$. For example, in a two-dimensional space, a hyperplane is a line.



Classification Problem

Feature space

- Space formed by the predictors
- Also referred to as the state space, input space
- p-dimensional (p predictors), n-points (n observations)

Training data

- Inputs determine the location in the feature space

$$x_1 = \begin{pmatrix} x_{11} \\ \vdots \\ x_{1p} \end{pmatrix}, \ldots, x_n = \begin{pmatrix} x_{n1} \\ \vdots \\ x_{np} \end{pmatrix}$$

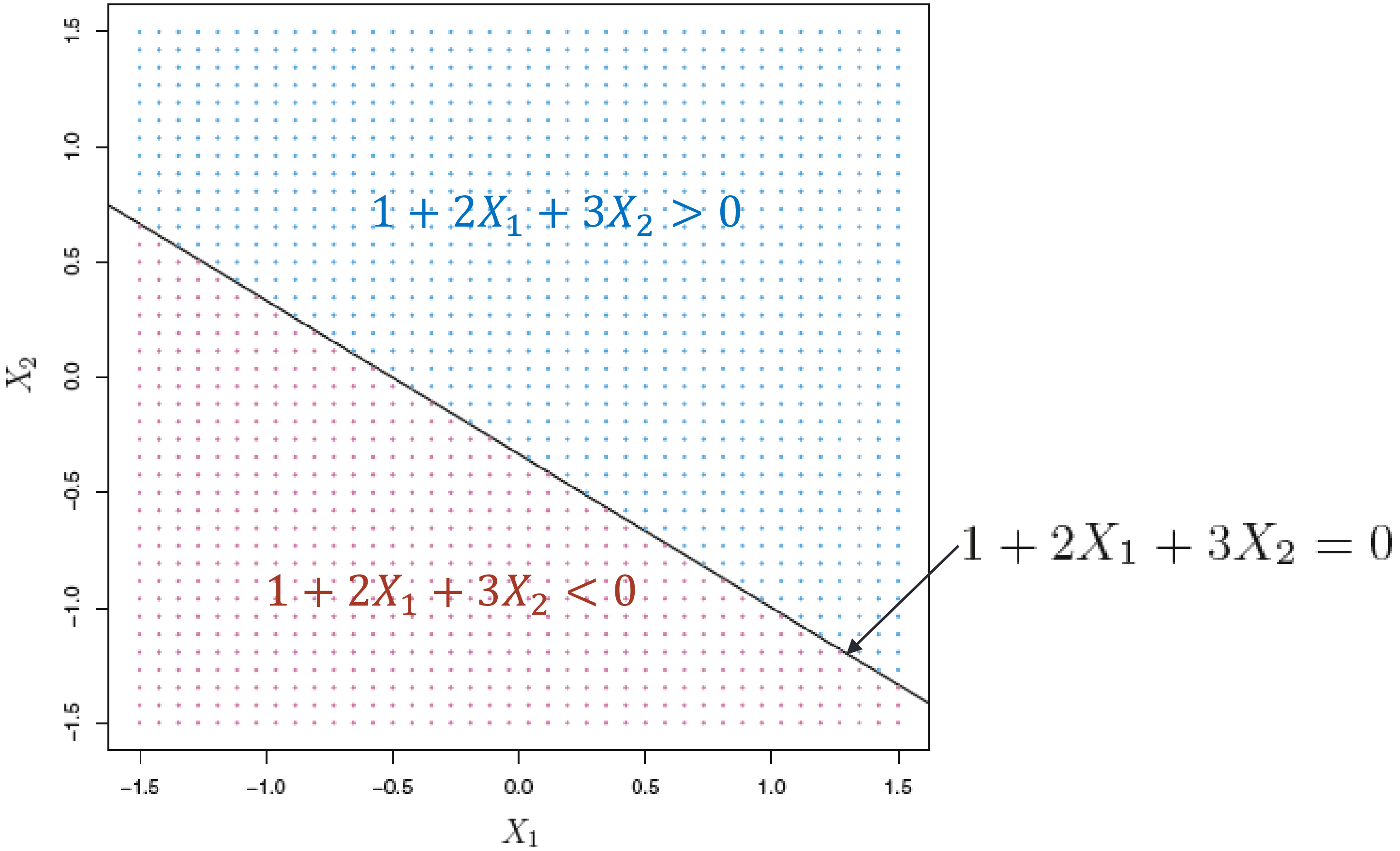
- Outputs $y_1, \ldots, y_n$ determine the **color** (i.e., **classes**)

Classification: <u>Find the hyperplane</u> such that a test point

$$x^* = \begin{pmatrix} x_1^* & \ldots & x_p^* \end{pmatrix}^T$$

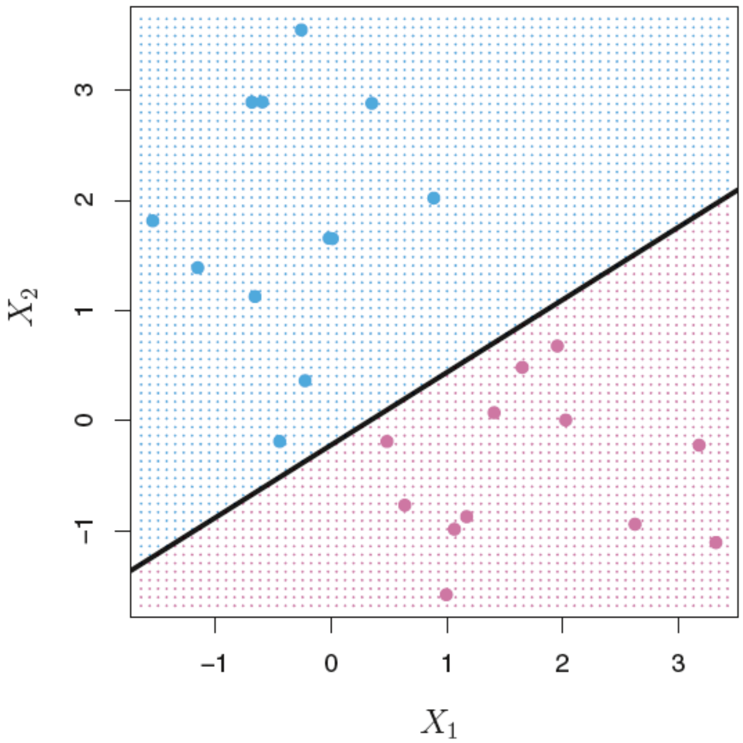
is assigned the correct class.

Classifier as Feature Space Coloring



Separating Hyperplane

- **Separating hyperplane**: separates the training observations perfectly according to their class labels
- Blue: class 1 ($y = 1$)
  Purple: class –1 ($y = -1$)



- $f(x) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_p x_p$
- class 1: $f(x) > 0$
  class –1: $f(x) < 0$

- Property: $\boldsymbol{y_i f(x_i) > 0}$, for all training points $x_1, x_2, \ldots, x_n$

Prediction

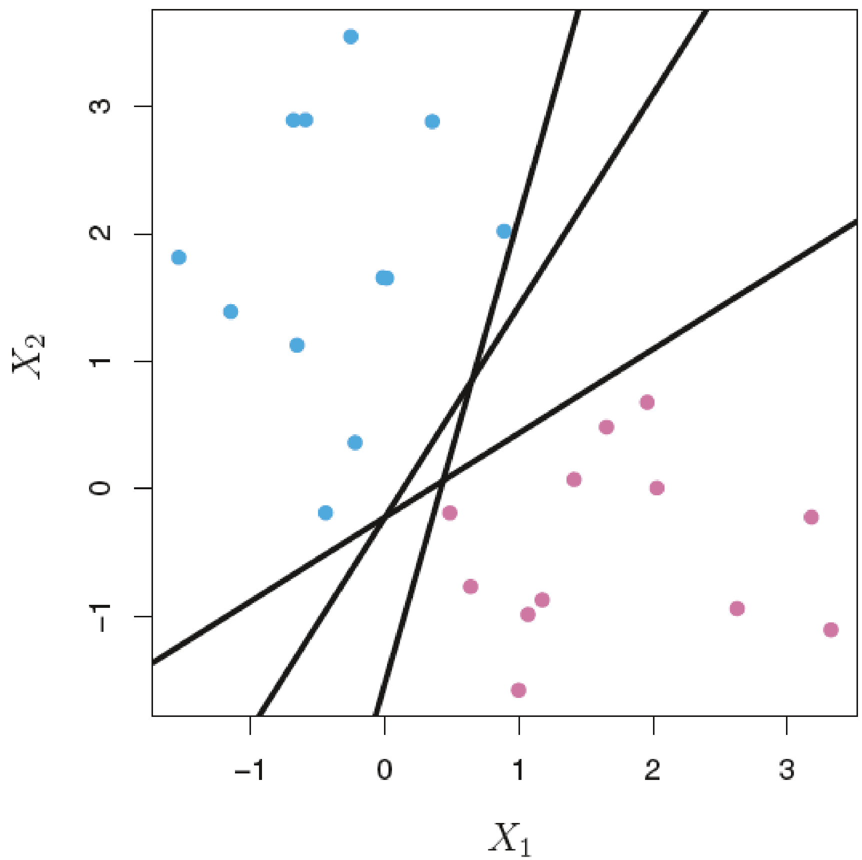
- Given a test point x^*, we will assign it to
  class 1 ($y^* = 1$), if $f(x^*) > 0$
  class –1 ($y^* = -1$), if $f(x^*) < 0$

- If $\boldsymbol{y^* f(x^*)}$ is far from zero, that means the test point lies far from the hyperplane, and so we can be confident about our class assignment for it.

- If $\boldsymbol{y^* f(x^*)}$ is close to zero, that means the test point is located near the hyperplane, and so we are less certain about the class assignment for it.

How to Do It Right?

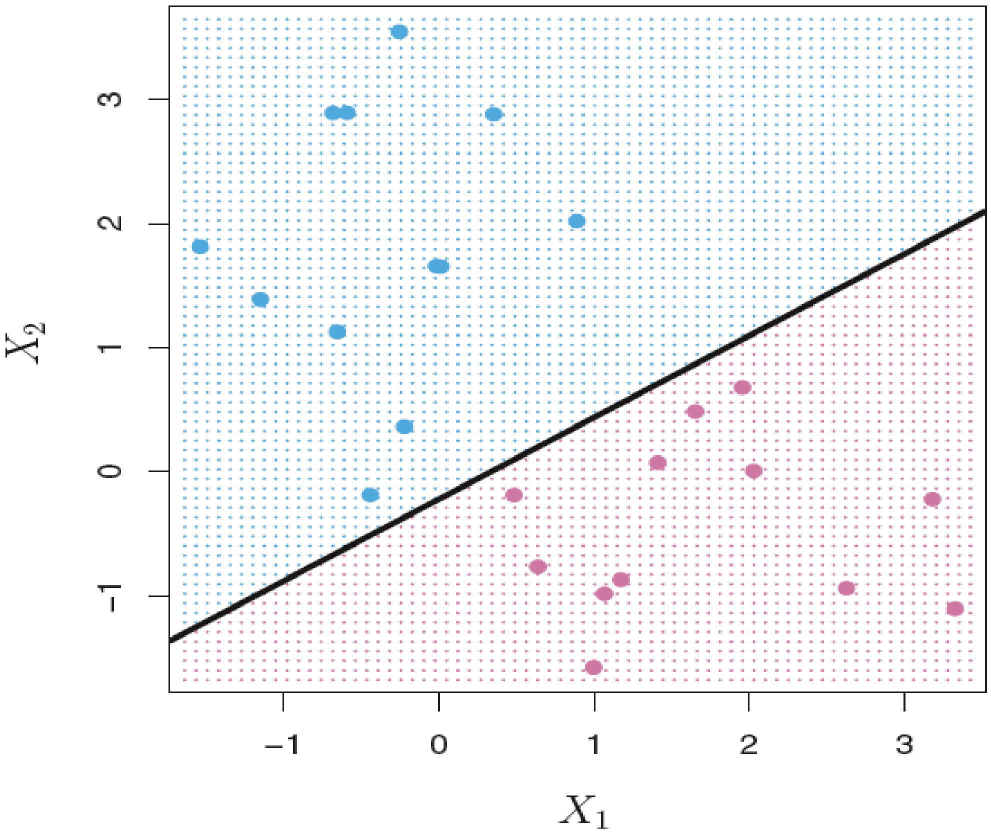
- There may be an infinite number of hyperplanes that separates the training observations perfectly.
- We need to decide which hyperplane to use.



Margin

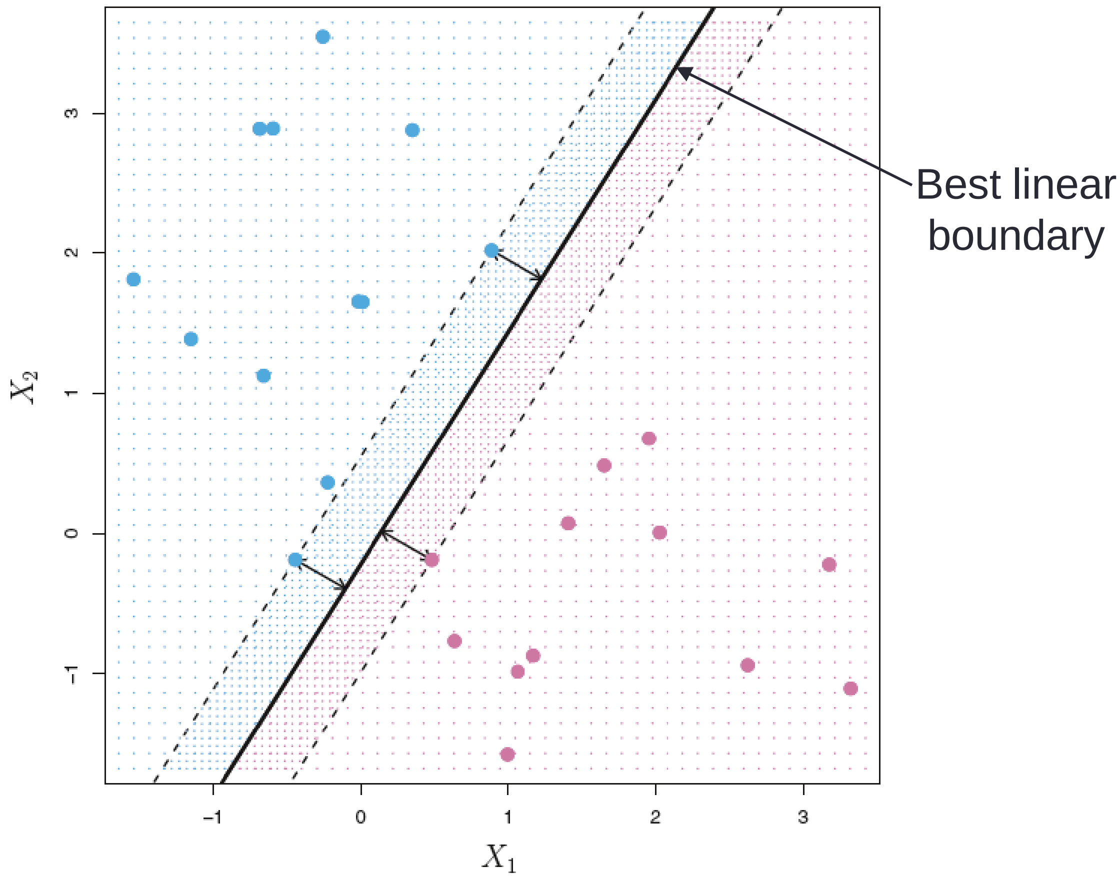
- Suppose we have a separating hyperplane
- Find perpendicular distance from every point to the hyperplane
- Margin: The smallest of such distances, M

  i.e., minimum distance from the observations to the hyperplane



Maximal Margin Classifier

- Best separating hyperplane
- Maximize min-distance (max margin)
- Represent the mid-line of the widest “slab” inserted between the two classes



Support Vectors

- Support vectors: the 3 training points equidistant from the maximal margin hyperplane
  - "vectors": each point is a vector in p-dimensional space
  - "support": they support the maximal margin hyperplane: if they were moved slightly then the maximal margin hyperplane would move as well.

- The maximal margin hyperplane depends directly on the support vectors, but not on the other observations: a movement of any of those observations would not affect the separating hyperplane.

Optimization Formulation

$$\underset{\beta_0,\beta_1,\ldots,\beta_p}{\text{maximize}}\, M$$

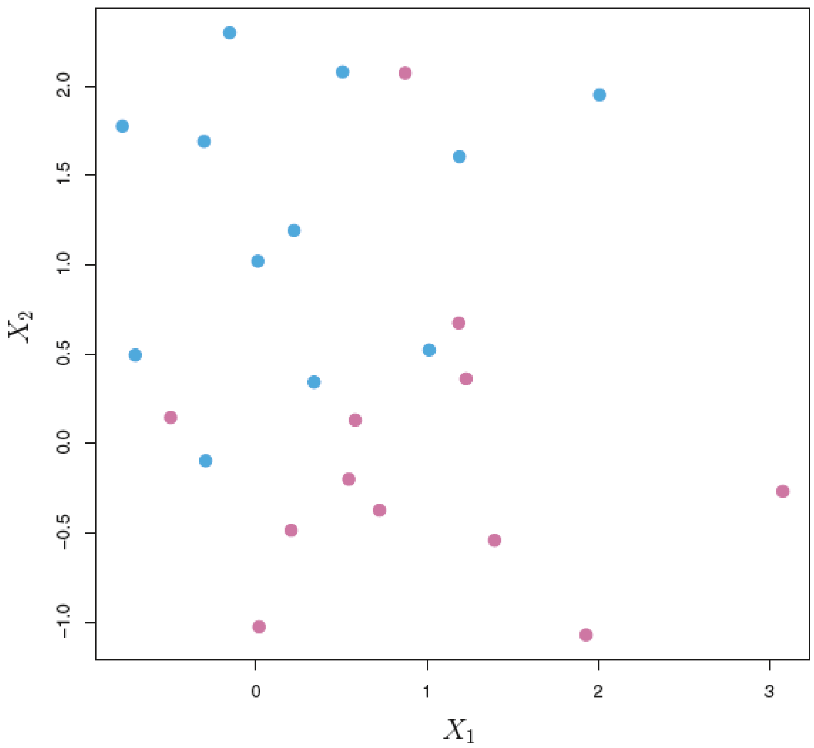
$$\text{subject to } \sum_{j=1}^{p} \beta_j^2 = 1,$$

$$y_i(\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \ldots + \beta_p x_{ip}) \geq M \quad \forall\ i = 1, \ldots, n$$

Question: for each point to be on the correct side of the hyperplane, we only need $y_i f(x_i) > 0$. Why here it is required that $y_i f(x_i) > M$ $(M > 0)$?

Non-separable Case

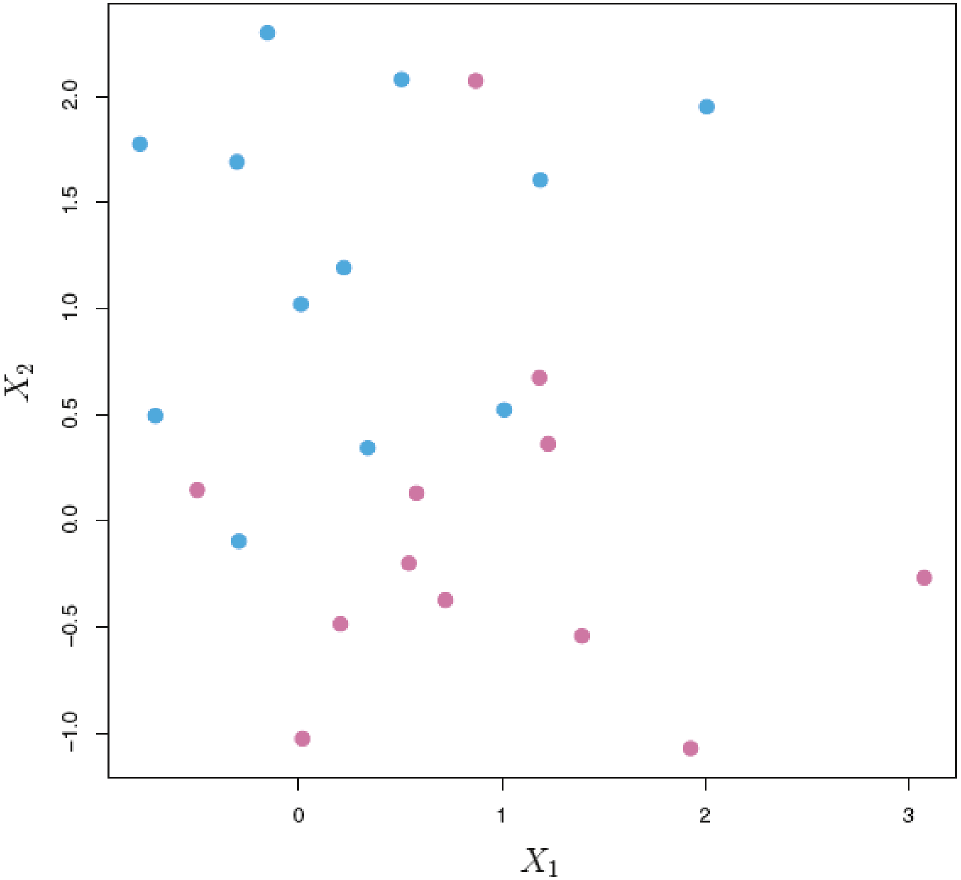
- No solution if the observation classes are mixed (*non-separable* case)
- We can extend the concept of a separating hyperplane to develop a hyperplane that almost separate the classes, using the idea of "soft margin"
- This generalization to the non-separable case is known as the **support vector classifier**



Support Vector Classifier

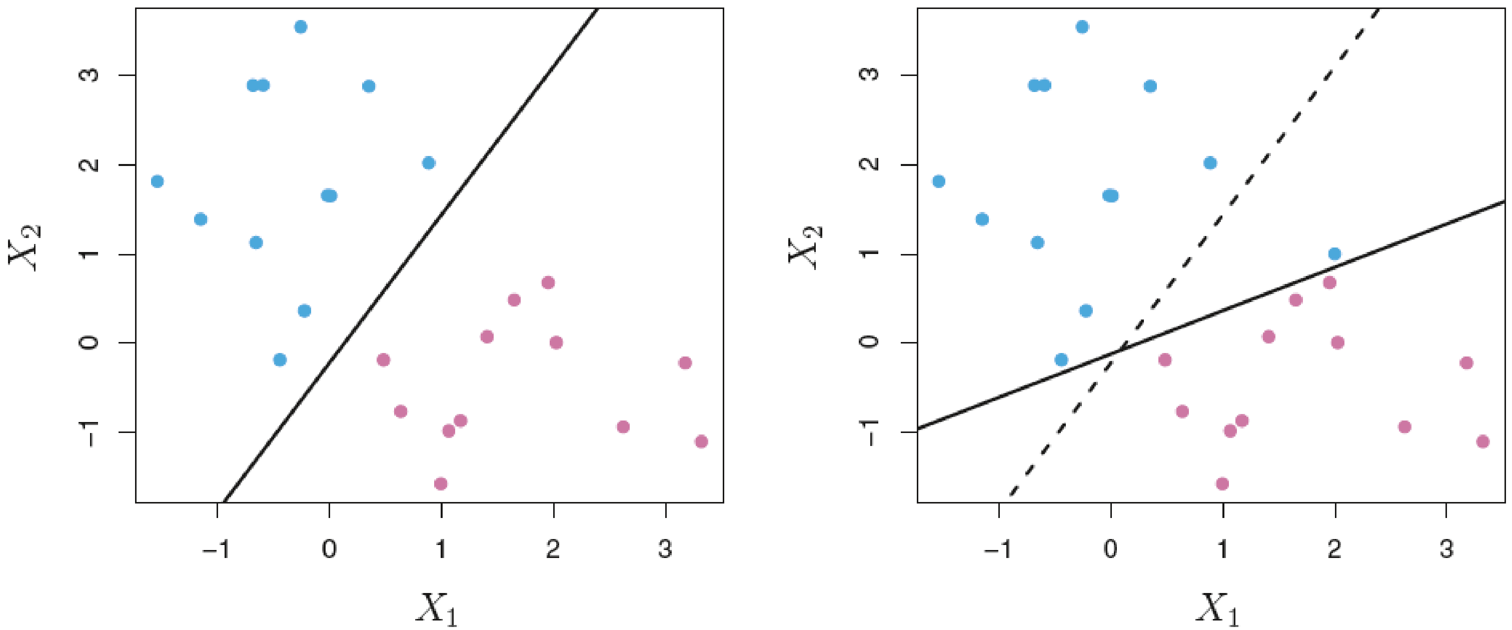
Motivation

- Maximal margin classifier only works for separable cases
- Need to extend it to the non-separable case



Motivation

- In the separable case, the separating hyperplane is sensitive to individual observations.
- The addition of a single observation may lead to dramatic change in the maximal margin hyperplane.
- Reason: margin is tiny (recall that $yf(x)$ is a measure of our confidence of correct classification)



Idea of Support Vector Classifier

- Consider a hyperplane that does not perfectly separate the two classes, in the interest of

  Greater robustness to individual observations, and

  Better classification of most of the training observations

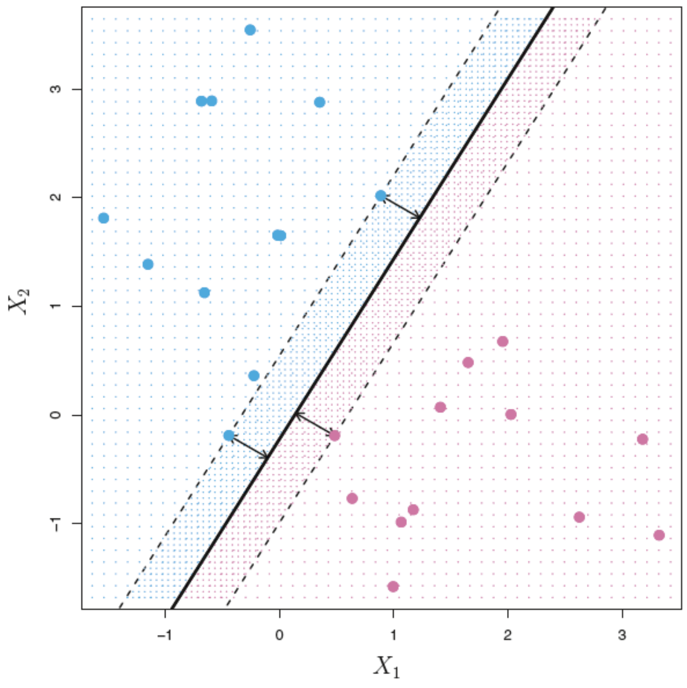
- It could be worthwhile to misclassify a few training points in order to do a better job in classifying the remaining points.

- Soft margin classifier: the margin is "soft" because it can be violated by some of the training points.

Idea of Support Vector Classifier

- Rather than seeking the largest possible margin so that every observation is not only on the correct side of the hyperplane but also on the correct side of the margin, we instead allow some observations to be on the incorrect side of the margin, or even the incorrect side of the hyperplane.

- An observation can be not only on the wrong side of the margin, but also on the wrong side of the hyperplane. Observations on the wrong side of the hyperplane correspond to training observations that are misclassified by the support vector classifier.



Relax the Constraint of Perfect Separation

- Support vector classifier

$$\underset{\beta_0,\beta_1,\ldots,\beta_p,\epsilon_1,\ldots,\epsilon_n}{\text{maximize}} \quad M$$

$$\text{subject to } \sum_{j=1}^{p} \beta_j^2 = 1,$$

$$y_i(\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_p x_{ip}) \geq M(1 - \epsilon_i)$$

$$\epsilon_i \geq 0, \quad \sum_{i=1}^{n} \epsilon_i \leq C,$$

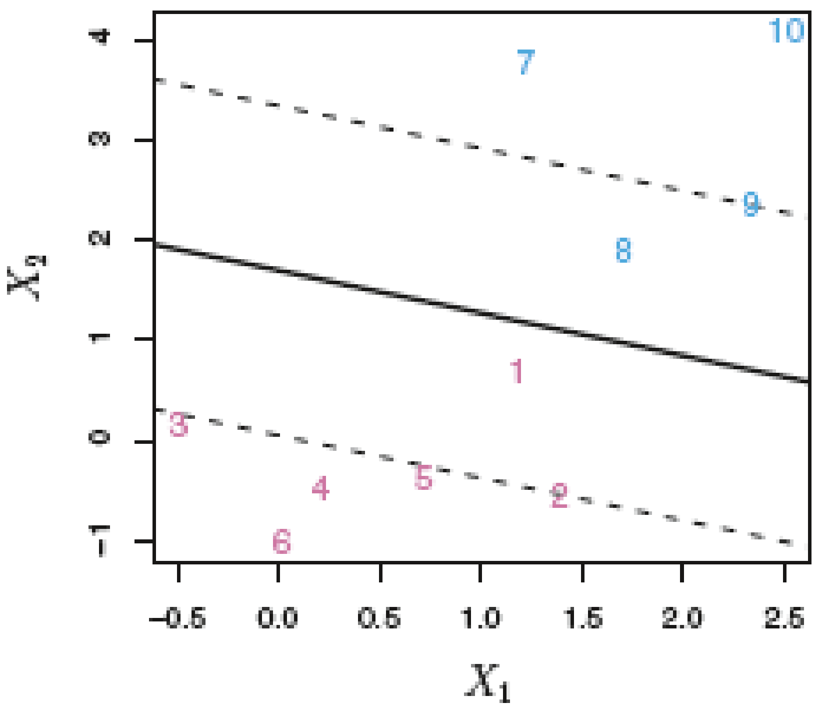
$\epsilon_1, \epsilon_2, \ldots, \epsilon_n$ are slack variables that allow individual observations to be on the wrong side of the margin or the hyperplane.

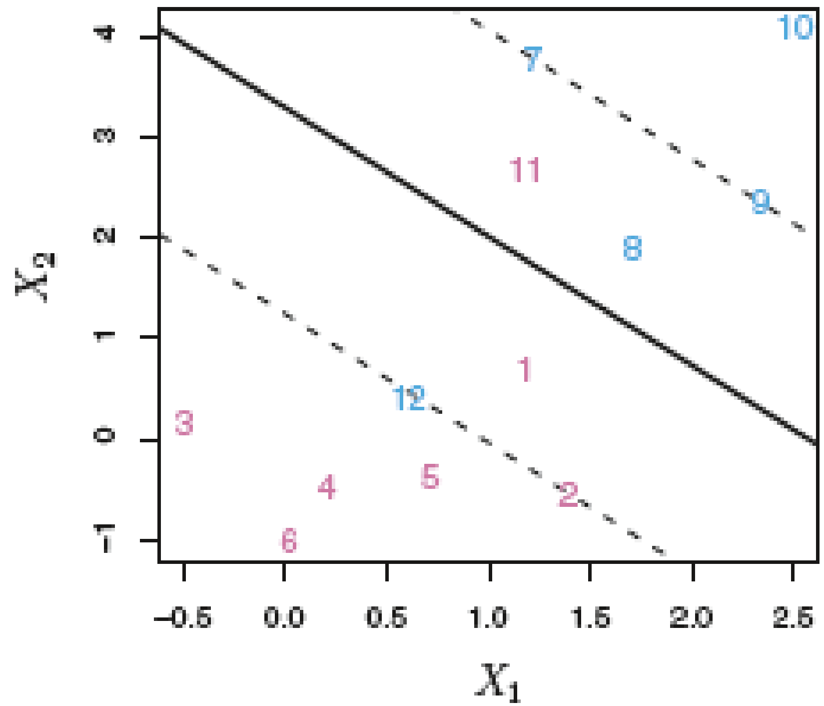
Slack Variables and Tuning Parameter

- For a sample i,
  - $\epsilon_i = 0$ margin not violated (on the correct side of the margin)
  - $\epsilon_i > 0$ margin violated (on the wrong side of the margin)
  - $\epsilon_i > 1$ hyperplane boundary crossed (on the wrong side of the hyperplane, or leakage)

  C: tuning parameter, a budget for the amount that the margin can be violated

Effect of ϵ





3,4,5,6: on the correct side of the margin
2: on the margin
1: on the wrong side of the margin

7,10: on the correct side of the margin
9: on the margin
8: on the wrong side of the margin

11,12: on the wrong side of the margin and the wrong side of the hyperplane

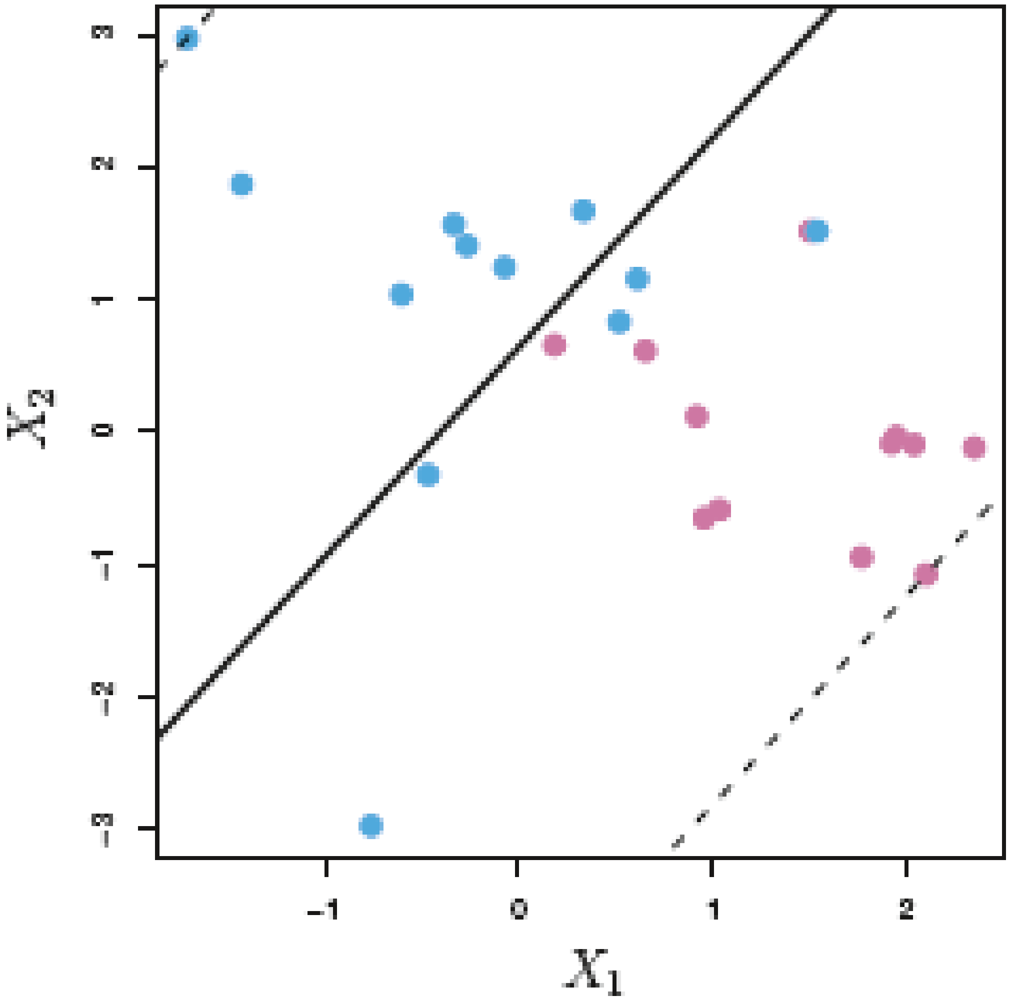
Effect of *C* — Bias-Variance Trade-off

- Small C
  - Narrow margins
  - Rarely violated
  - Fitting data well
  - Low bias but high variance

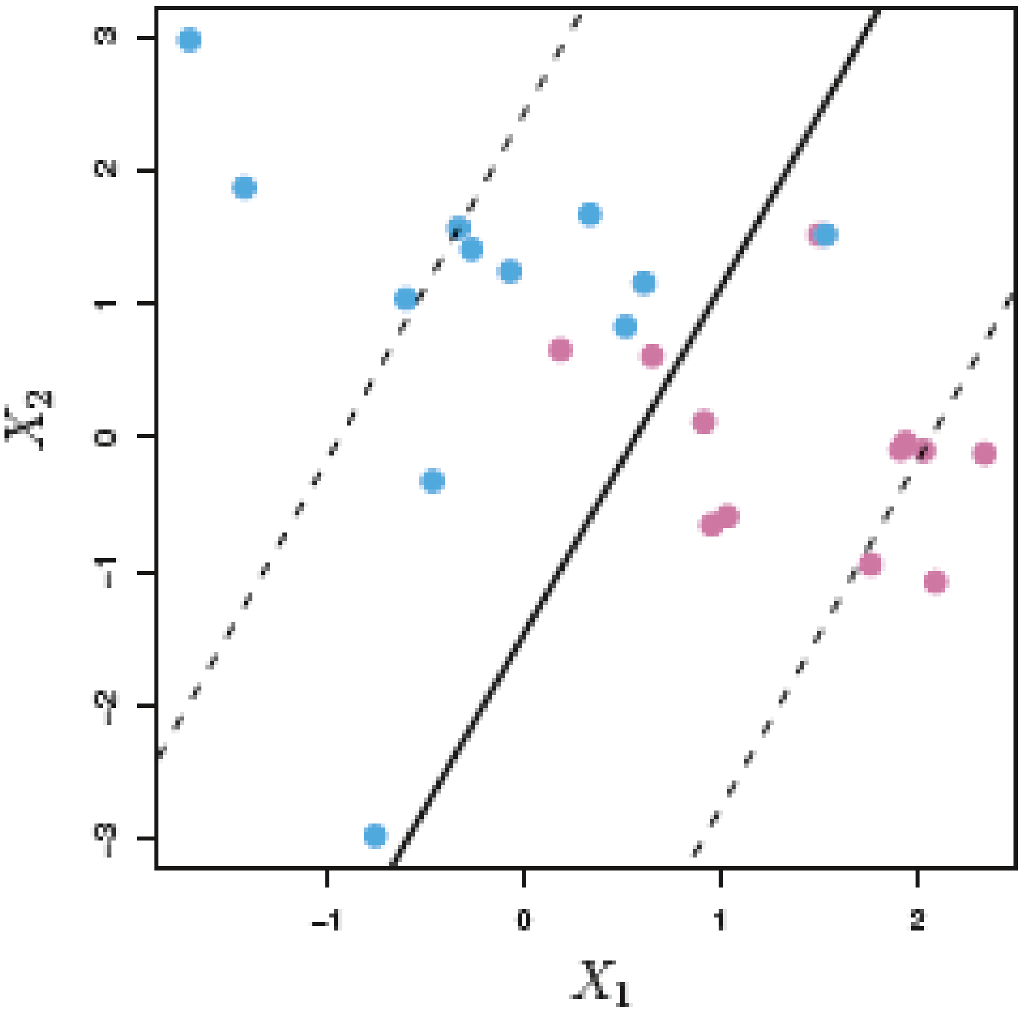
- Large C
  - Wide margins
  - Allow more violations
  - Fitting data less hard
  - Low variance but high bias

- In practice, C is treated as a tuning parameter and chosen via cross validation.

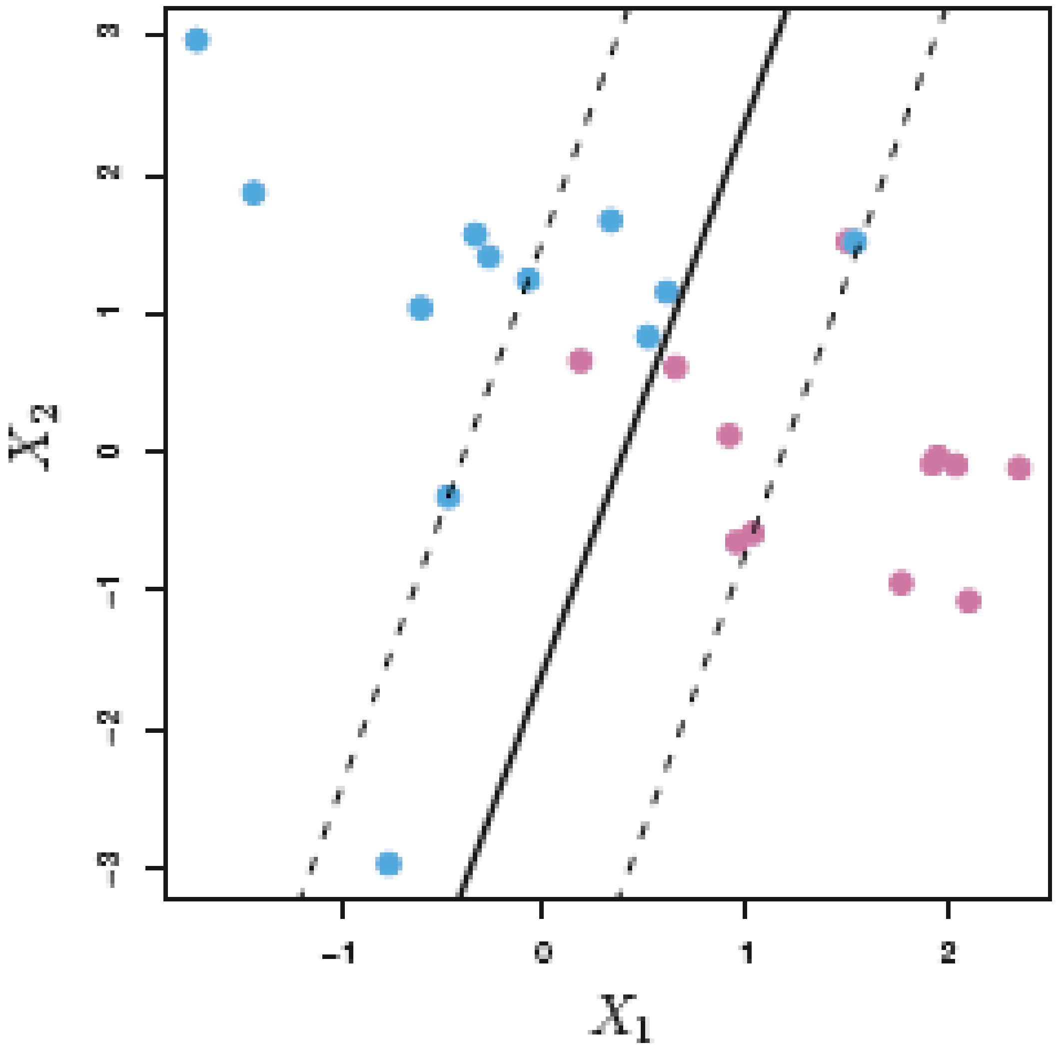
$C = 25$



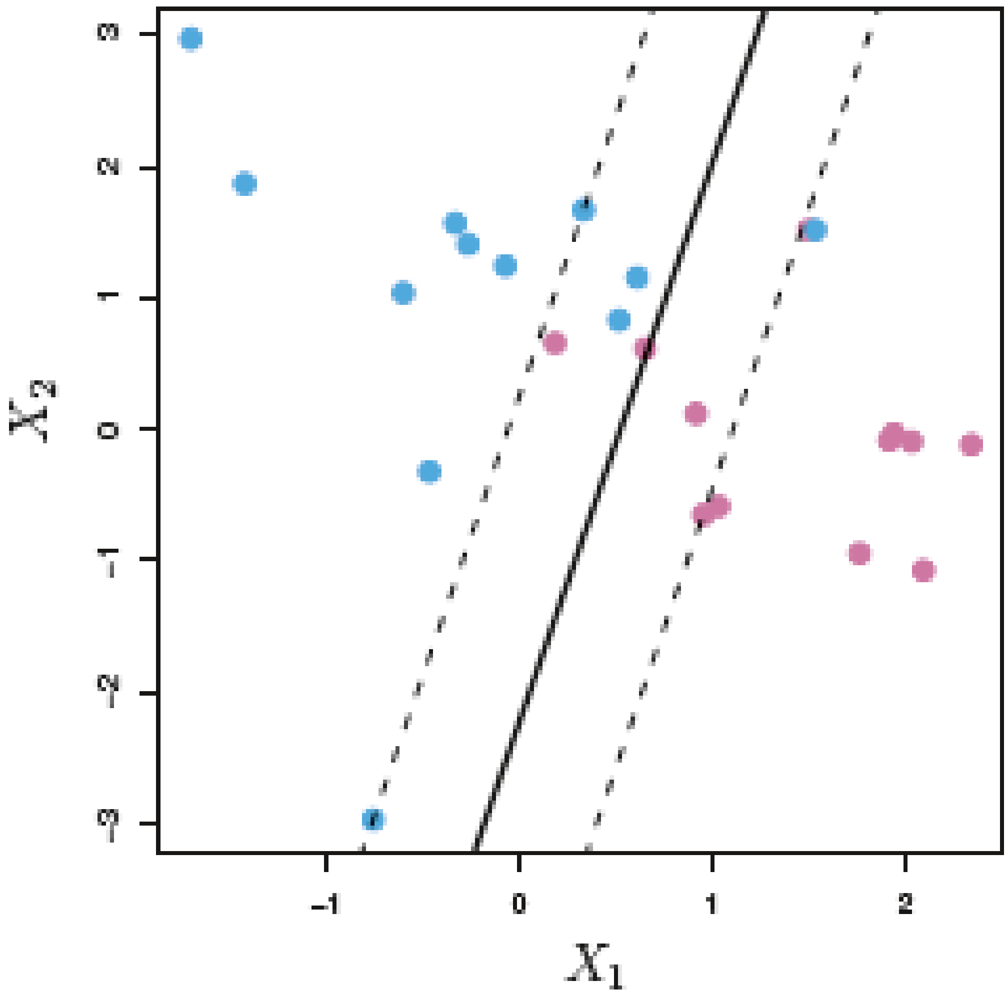
$C = 15$



$C = 10$



$C = 5$



Properties of the Solution to the Relaxed Formulation

- For the support vector classifier formulation, we have n constraints

$$y_i(\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_p x_{ip}) \geq M(1 - \epsilon_i)$$

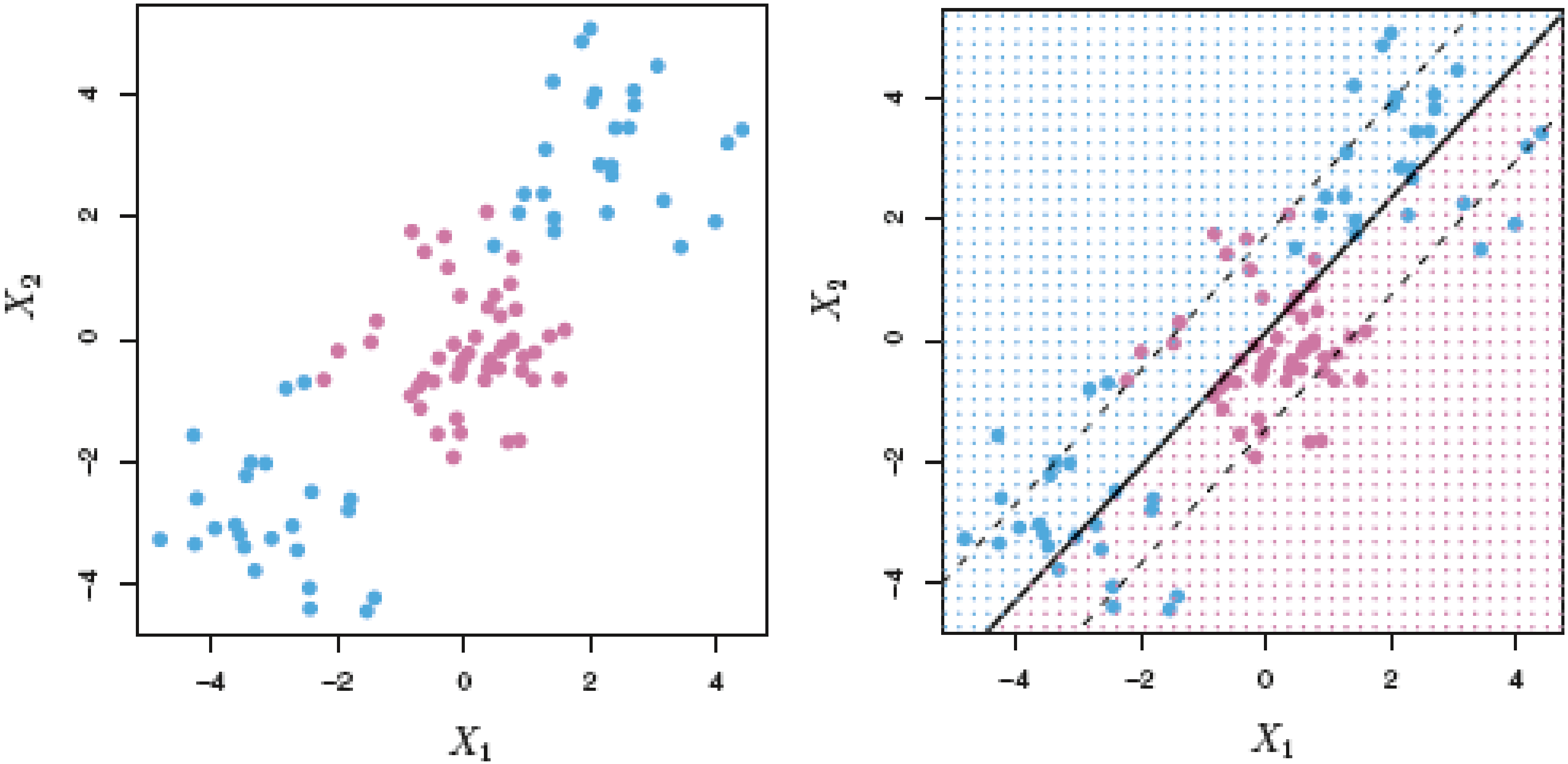
- Support vectors: Points that lie on the margin or on the wrong side of the margin for their class (including those on the wrong side of the hyperplane)

- Observations that lie strictly on the correct side of the margin do not affect the support vector classifier.

Support Vector Machine

Motivation

- What would you use to classify?
- Linear classifier performs poorly.



Accommodating Nonlinearity

- Recall Chapter 3: linear regression may suffer when there is nonlinear relationship between predictors and the response. The solution is to add *transformations* (e.g., quadratic and cubic terms) of predictors into the model. Similar idea can be applied here.

- Instead of fitting a support vector classifier using the p features $X_1, X_2, \dots, X_p$, we can enlarge the feature space by using $X_1, X_1^2, X_2, X_2^2 \dots, X_p, X_p^2$.

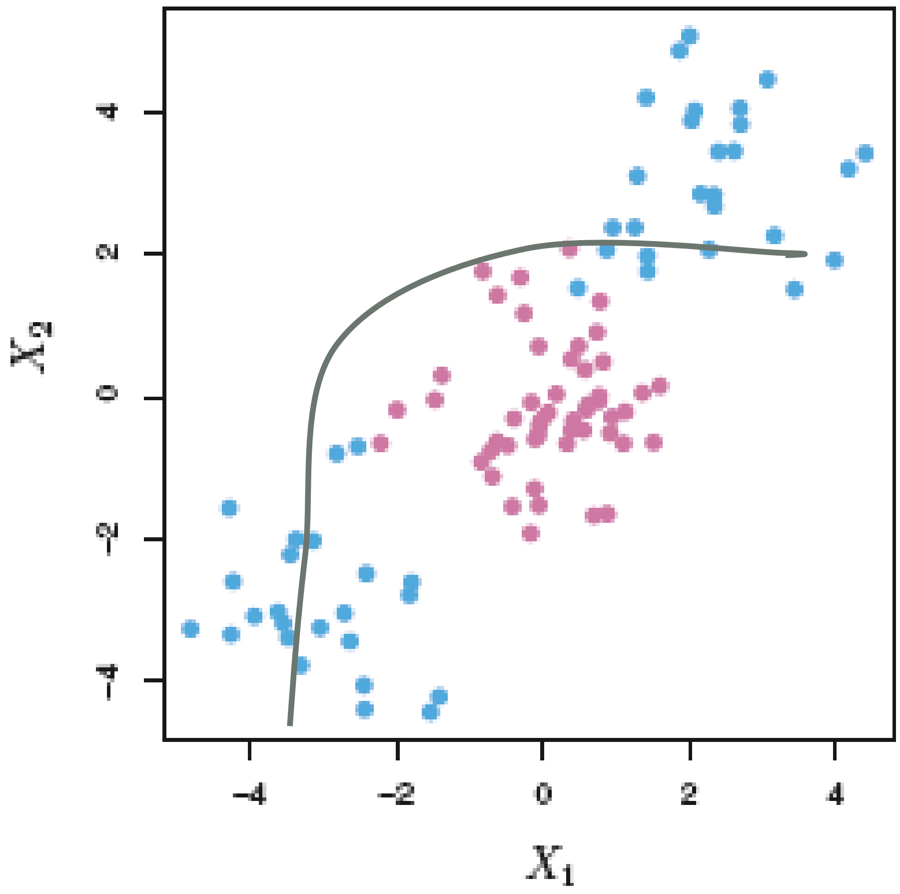
Modified Optimization Formulation

$$\underset{\beta_0,\beta_{11},\beta_{12},\ldots,\beta_{p1},\beta_{p2},\epsilon_1,\ldots,\epsilon_n}{\text{maximize}} \quad M$$

$$\text{subject to } y_i\left(\beta_0 + \sum_{j=1}^{p}\beta_{j1}x_{ij} + \sum_{j=1}^{p}\beta_{j2}x_{ij}^2\right) \geq M(1-\epsilon_i)$$

$$\sum_{i=1}^{n}\epsilon_i \leq C, \quad \epsilon_i \geq 0, \quad \sum_{j=1}^{p}\sum_{k=1}^{2}\beta_{jk}^2 = 1.$$

Example



However…

- Including quadratic terms is only one way to enlarge the feature space in order to accommodate nonlinearity.
- There are many possible ways to enlarge the feature space. Unless we are careful, we could end up with a huge number of features. Then computations would become unmanageable.
- The support vector machine allows us to enlarge the feature space in a way that leads to efficient computations.

Properties of Optimal Hyperplane

- Let us define an inner product (dot product) of two vectors:

$$\langle a, b \rangle = \sum_{i=1}^{r} a_i b_i$$

For real vectors, it is simply $a^T b$.

- The optimal linear hyperplane $f(x) = 0$ can be written as

$$f(x) = \beta_0 + \sum_{i=1}^{n} \alpha_i \langle x, x_i \rangle$$

It turns out that $\alpha_i \neq 0$ only for support vectors

$$f(x) = \beta_0 + \sum_{i \in \mathcal{S}} \alpha_i \langle x, x_i \rangle.$$

- **Decision rule is based on the inner product**.

Support Vector Machine (SVM)

- Let us generalize the support vector classifier

$$f(x) = \beta_0 + \sum_{i \in \mathcal{S}} \alpha_i \langle x, x_i \rangle$$

$$\downarrow$$

$$f(x) = \beta_0 + \sum_{i \in \mathcal{S}} \alpha_i K(x, x_i)$$

$K(\cdot,\cdot)$ is called the *kernel* (function), which is a function that quantifies the similarity of two observations.

Choices of Kernel Function

- Linear kernel (i.e., support vector classifier)

$$K(x_i, x_{i'}) = \sum_{j=1}^{p} x_{ij} x_{i'j}$$

- Polynomial kernel

$$K(x_i, x_{i'}) = (1 + \sum_{j=1}^{p} x_{ij} x_{i'j})^d$$

tuning parameter: d

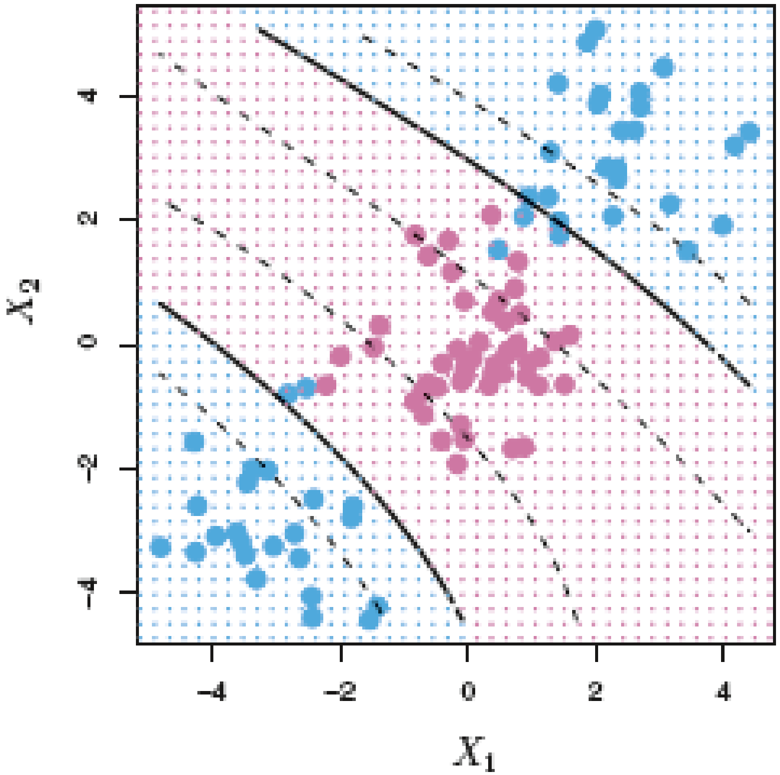
- Radial kernel

$$K(x_i, x_{i'}) = \exp(-\gamma \sum_{j=1}^{p} (x_{ij} - x_{i'j})^2)$$

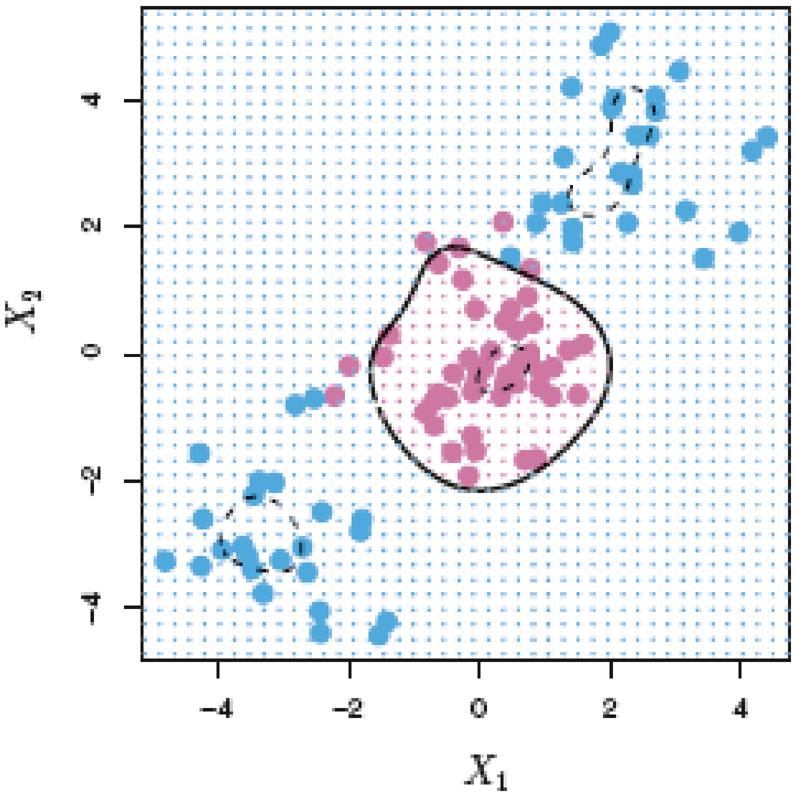
tuning parameter: γ

SVM Boundaries

Degree 3 polynomial kernel



Radial kernel



Advantage of Using Kernel

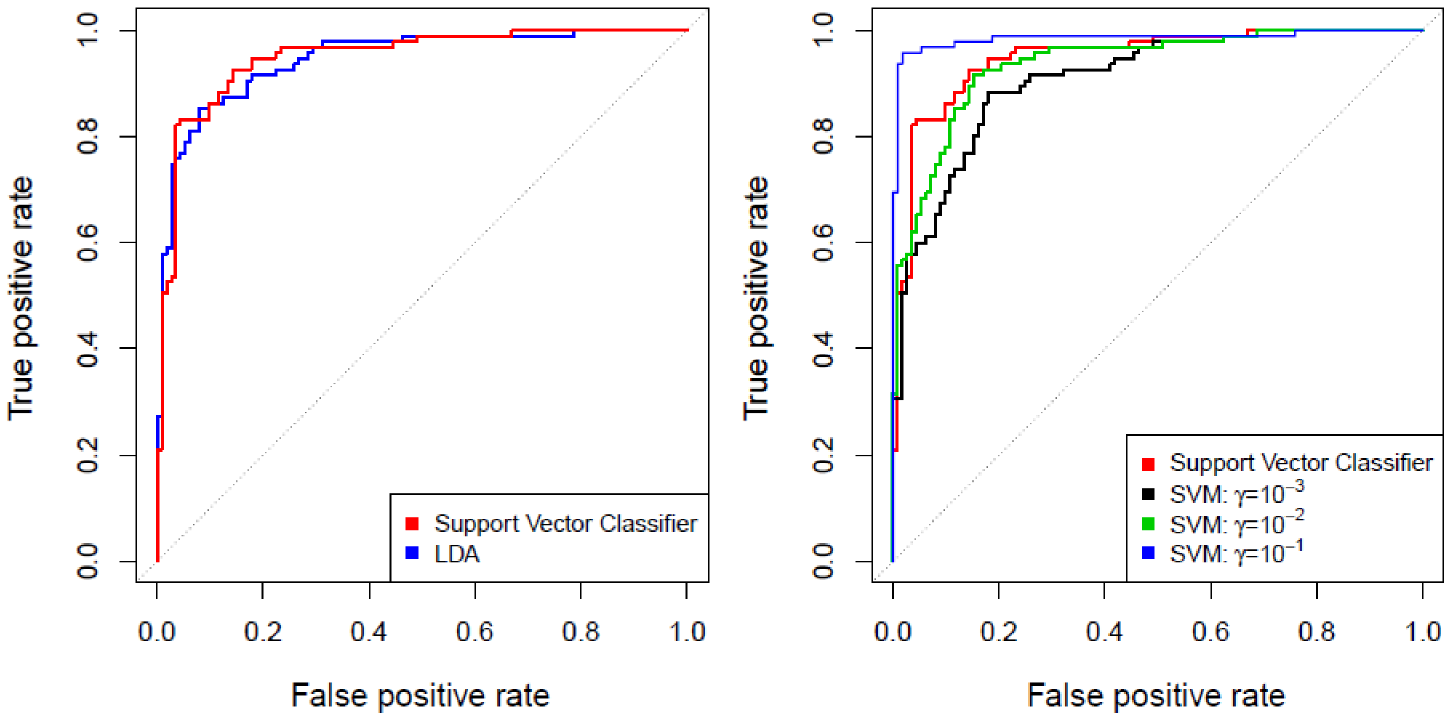
- We use a kernel rather than simply enlarge the feature space using functions of the original features.

- There is advantage on computation. Using kernel, we only need to compute the kernel $K(x_i, x_{i'})$ for $\binom{n}{2}$ distinct pairs $x_i, x_{i'}$. This can be done without explicitly working in the enlarged feature space.

- This is important because in many applications of SVMs, the enlarged feature space is so large that computations are intractable. For some kernels, such as the radial kernel, the feature space is implicit and infinite-dimensional, so we could never do the computations there anyway!

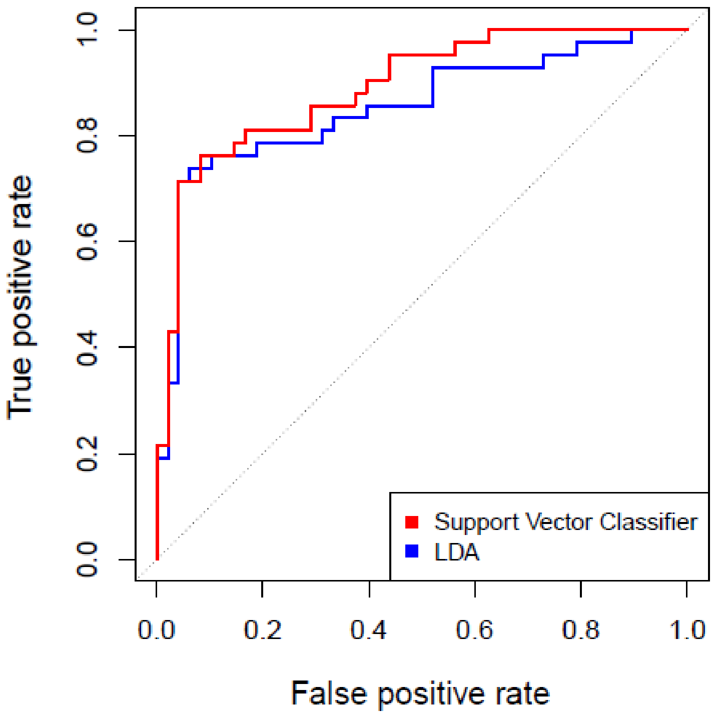
Example: Heart Disease Data

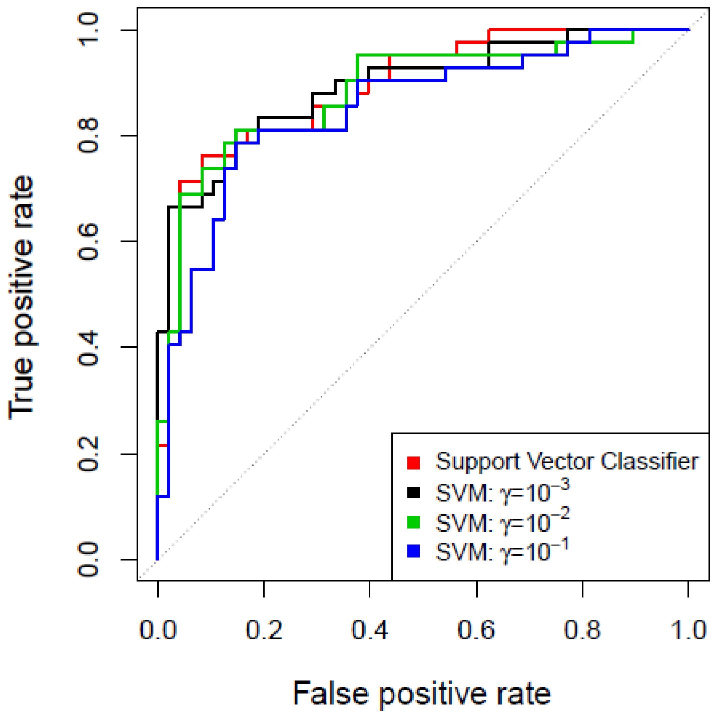
- ROC curves of LDA vs. SVM in training



Example: Heart Disease Data

- ROC curves of LDA vs. SVM in testing





Summary

- Maximal Margin Classifier
  linear boundary
  separable cases

- Support Vector Classifier
  linear boundary
  separable or non-separable cases
  (A special case of SVM when linear kernel is used.)

- Support Vector Machine
  linear or nonlinear boundary
  separable or non-separable cases

Questions (1)

Read slides of Topic 7. Then answer the following questions.

- What kind of problems is support vector machines used for?
- What is margin?
- What is maximal margin classifier?
- What are support vectors of maximal margin classifier?
- What is the situation the maximal margin classifier designed for?

Questions (2)

- What is the situation the support vector classifier designed for?
- What is soft margin?
- What is the effect of the tuning parameter C?
- How to find the optimal value of the tuning parameter?
- What are support vectors of support vector classifier?

Questions (3)

- What is the situation of SVM designed for?
- What are the choices of kernel functions in SVM?
- In using SVM with linear kernel, what is the tuning parameter?
- In using SVM with polynomial kernel, what are the tuning parameters?
- In using SVM with radial kernel, what are the tuning parameters?
- What is the relationship of maximal margin classier, support vector classifier, and SVM?