Chapter 9: Support Vector Machines

Support Vector Machines

- ▶ Developed in the 1990s
- ▶ One of the best "out of the box" classifiers

Outline

- Maximal Margin Classifier (SVMs are a generalization of MMCs)
- Support Vector Classifier (extension of MMCs to non-separable cases)
- Support Vector Machines (further extension of SVCs to accommodate non-linear boundaries)

Hyperplane

Hyperplane: a flat affine subspace of dimension p-1. (Subspace need not pass through the origin).

In 2-D: a flat one-dimensional subspace (a line)

$$\beta_0 + \beta_1 X_1 + \beta_2 X_2 = 0$$

In 3-D: a flat two-dimensional subspace (a plane)

$$\beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3 = 0$$

In p-D: difficult to visualize

$$\beta_0 + \beta_1 X_1 + \beta_2 X_2 + \dots + \beta_p X_p = 0$$

Hyperplane

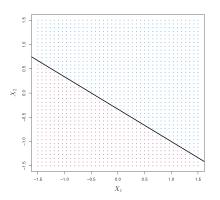


Figure 1: ISL 9.1

$$1 + 2X_1 + 3X_2 = 0$$

blue points:

$$1 + 2X_1 + 3X_2 > 0$$

Separating Hyperplanes

We can use a separating hyperplane to construct a classifier: a test observation is assigned a class depending on which side of the hyperplane it is located.

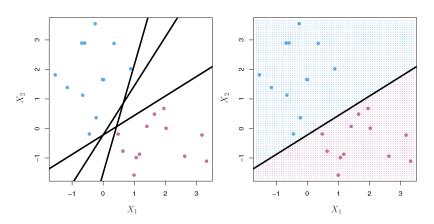


Figure 2: ISL 9.2

Maximal Margin Classifier

If the data can be linearly separated, infinite possible hyperplanes exist.

The *maximal margin hyperplane* is the separating hyperplane that is farthest from the training observations (has the largest *margin*).

(We compute the distance from each observation to the hyperplane and consider the smallest distance as the *margin*.)

A classifier based on this hyperplane is the maximal margin classifier.

Maximal Margin Classifier

Support vectors are vectors in p-dimensional space that 'support' the maximal margin hyperplane. The maximal margin hyperplane depends only on a subset of observations.

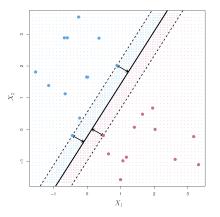


Figure 3: ISL 9.3

Maximal Margin Classifier

The maximal margin classifier is the solution to:

$$\begin{aligned} & \underset{\beta_0,\beta_1,...,\beta_p,M}{\text{maximize }} M \\ & \text{subject to } \sum_{j=1}^p \beta_j^2 = 1, \\ & y_i(\beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + ... + \beta_p X_{ip}) \geq M \ \forall \ i = 1,...,n \end{aligned}$$

where M is the margin of the hyperplane and $y_i,...,y_n \in \{-1,1\}$

Using a *soft-margin*, we can identify a hyperplane that *almost* separates the classes. This can be desirable if

- 1. No separating hyperplane exists.
- 2. We want to reduce sensitivity to individual observations.

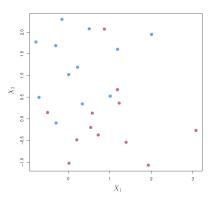


Figure 4: ISL 9.4

The support vector classifier is the solution to:

$$\begin{aligned} & \underset{\beta_0,\beta_1,...,\beta_p,\epsilon_1,...,\epsilon_n,M}{\text{maximize}} M \\ & \text{subject to} \sum_{j=1}^p \beta_j^2 = 1, \\ & y_i(\beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + ... + \beta_p X_{ip}) \geq M(1 - \epsilon_i) \\ & \epsilon_i \geq 0, \sum_{i=1}^n \epsilon_i \leq C, \end{aligned}$$

where C is a nonnegative tuning parameter and $\epsilon_1, ..., \epsilon_n$ are slack variables that allow individual observations to be on the wrong side of the margin or the hyperplane.

- $\epsilon_i = 0$: *i*th observation on correct side of **margin**
- $\epsilon_i > 0$: *i*th observation on wrong side of **margin**
- $\epsilon_i > 1$: *i*th observation on wrong side of **hyperplane**

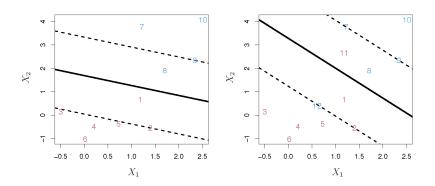


Figure 5: ISL 9.6

What happens as C increases?

Only the observations on the margin or on the wrong side of the margin (support vectors) will affect the hyperplane.

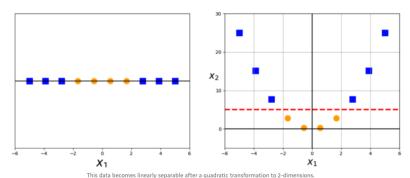
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Support Vector Machines

Use *kernels* to enlarge feature space and accommodate non-linear boundaries between the classes.



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Figure 7: 1-D to 2-D; D. Wilimitis

Support Vector Machines

Use *kernels* to enlarge feature space and accommodate non-linear boundaries between the classes.

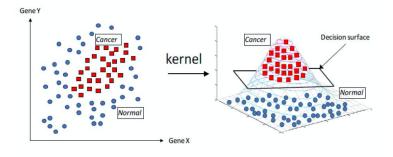


Figure 8: 2-D to 3-D; E. Mokshyna

Kernel

A function that quantifies the similarity of two observations.

$$K(x_i,x_{ij})$$

Kernel

The function for a support vector classifier can be written as

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

where S is the collection of indices of the support vectors

Linear Kernel

 Quantifies the similarity of a pair of observations using Pearson correlation

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

► This just gives us the Support Vector Classifier

Polynomial Kernel

► Fits a support vector classifier in higher-dimensional space involving polynomials of degree *d* rather than in the original feature space.

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

► An SVC with a non-linear kernel such as the polynomial kernel is known as a support vector machine.

Polynomial Kernel

SVM with polynomial kernel of degree 3:

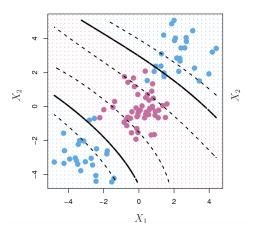


Figure 9: ISL 9.9

Radial Kernel

Another non-linear kernel is the radial kernel:

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

Radial Kernel

SVM with radial kernel:

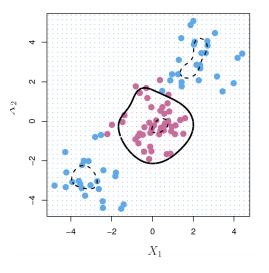


Figure 10: ISL 9.9

SVMs with >2 classes

- ▶ One-vs-one: construct $\binom{K}{2}$ SVMs, each of which compares a pair of classifiers
- ▶ One-vs-all: construct K SVMs, each of which compares the kth class to all others.

Summary

- ► SVMs use a kernel function to enlarge the feature space and accommodate non-linear class boundaries.
- Linear, polynomial, and radial kernels can be used.