DSO530 Statistical Learning Methods

Lecture 8 : Support Vector Machines (SVMs)

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Introduction

- Topics include *maximal margin classifiers*, *support vector classifiers* and *support vector machine (SVM)*
- SVMs were invented in the 1990s; it had some dominance until the resurgence of neural networks.
- SVMs are still considered one of the best `off-the-shelf` classifiers
- People often loosely refer to the maximal margin classifier, the support vector classifier, and the support vector machine as "support vector machines"
- In SVM, people label the two classes by $+1$ and -1
- This lecture covers the methedology. For implementation, use `svm` in sklearn: https://scikit-learn.org/stable/modules/svm.html

Maximal margin classifier

- hyperplane: In a p-dimensional space, a hyperplane is a flat *affine* subspace of dimension $p - 1$
- *Affine* subspace is a fancy math term. It is like a linear subspace, but the origin is not necessarily in it
- Mathematically, a hyperplane is

$$\beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p = 0$$

- If $X = (X_1, \cdots, X_p)^T$ leads to $>$, it lies on one side of the hyperplane; if $<$, it lies on the other side

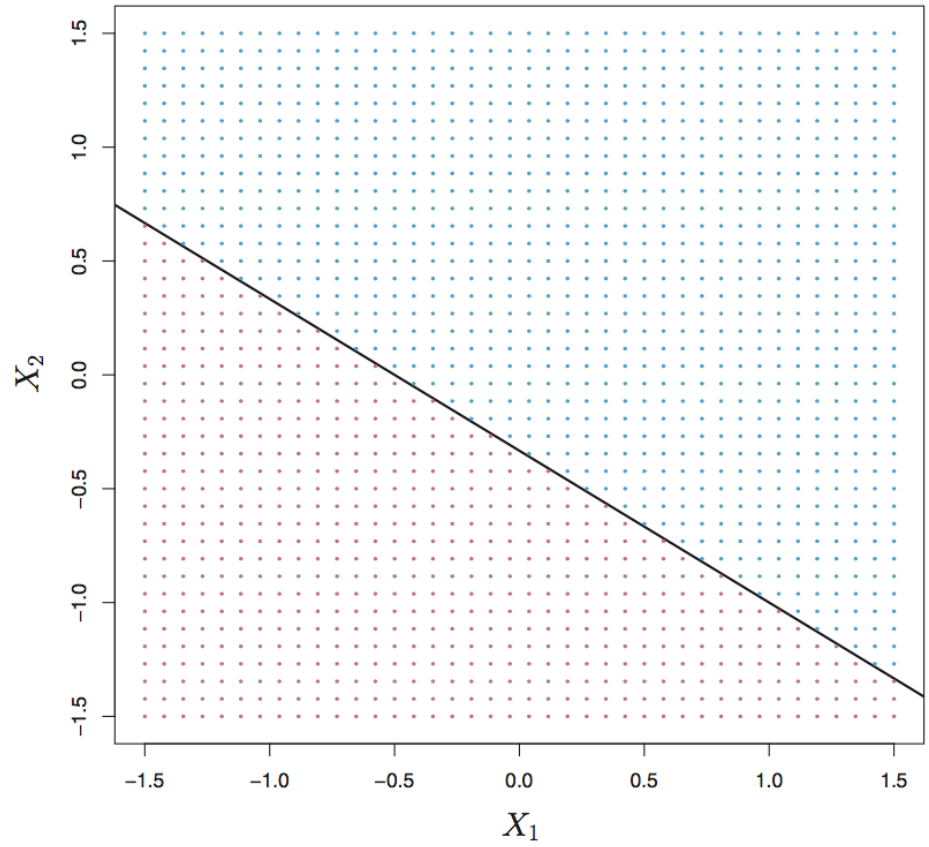


FIGURE 9.1. *The hyperplane* $1 + 2X_1 + 3X_2 = 0$ *is shown. The blue region is the set of points for which* $1 + 2X_1 + 3X_2 > 0$, *and the purple region is the set of points for which* $1 + 2X_1 + 3X_2 < 0$.

Figure 1

Classification Using a Separating Hyperplane

- Suppose that it is possible to construct a hyperplane that separates the training observations perfectly according to their class labels
- A separating hyperplane has the property that

$$y_i(\beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip}) > 0\,,$$

  for all $i = 1, \cdots, n$
- A test observation is assigned a class depending on which side of the hyperplane it is located
- That is, we classify the test observation x^* based on the sign of

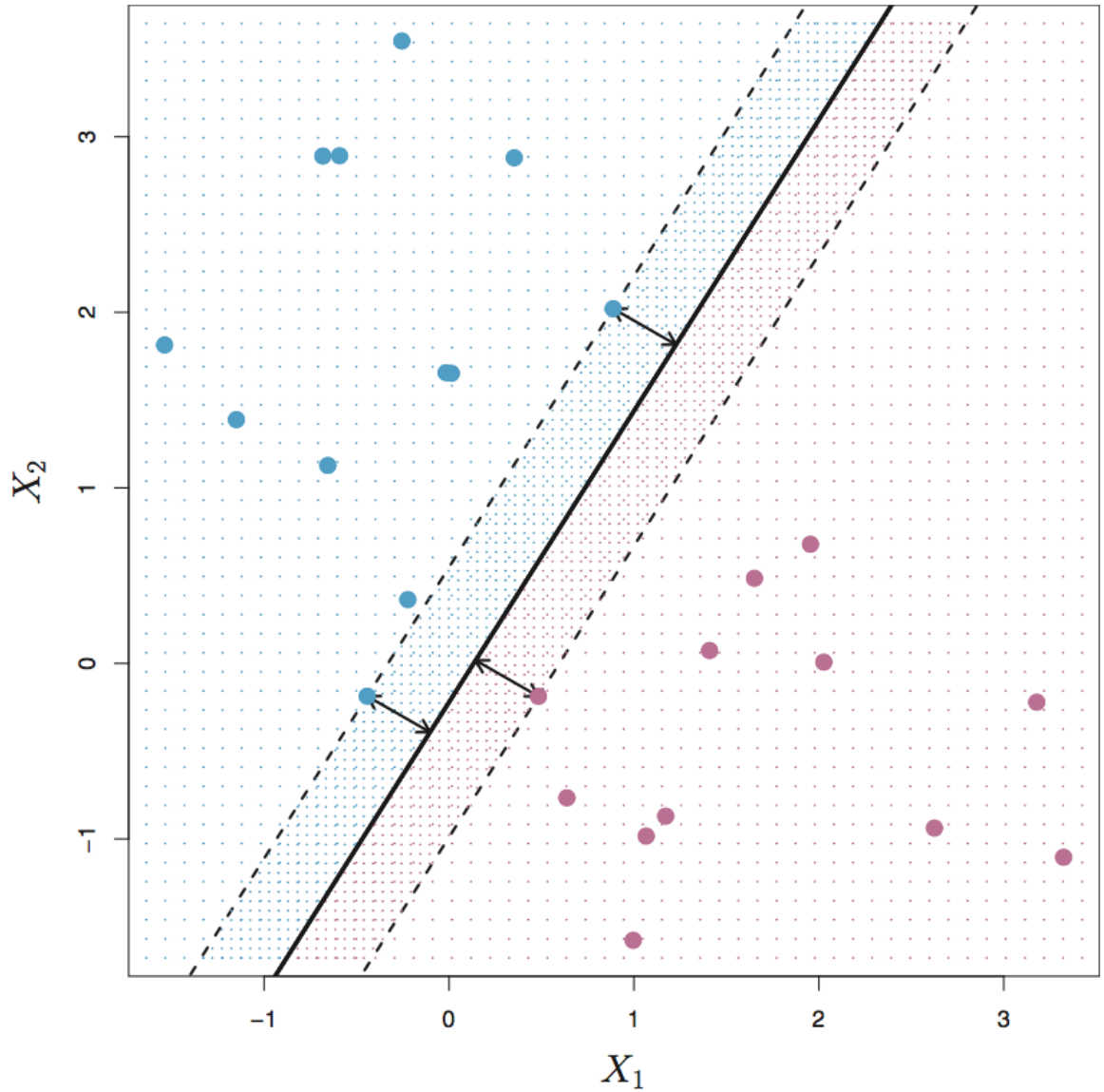
$$f(x^*) = \beta_0 + \beta_1 x_1^* + \cdots + \beta_p x_p^*$$

- If $f(x^*) > 0$, we assign to class 1, and if $f(x^*) < 0$, we assign to class -1
- In addition to the sign, how should you interpret $|f(x^*)|$?

The Maximal Margin Classifier

- If data can be perfectly separated by a hyperplane, then there exist an infinite number of such hyperplanes
- A natural question: which one do we want to choose?
- A natural choice is the maximal margin hyperplane (also known as the *optimal separating hyperplane*), which is the separating hyperplane that is farthest from the training observations.
- The minimal distance from the training observations to the hyperplane is known as the margin
- Maximal margin classifier: classify a test observation based on which side of the maximal margin hyperplane it lies

- There are three support vectors in the plot
- If you move other training data, what happens to the maximal margin classifier?



Construction of the Maximal Margin Classifier

$$\underset{\beta_0,\beta_1,\ldots,\beta_p,M}{\text{maximize}} \; M \tag{9.9}$$

$$\text{subject to} \sum_{j=1}^{p} \beta_j^2 = 1, \tag{9.10}$$

$$y_i(\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \ldots + \beta_p x_{ip}) \geq M \;\; \forall \, i = 1, \ldots, n. \tag{9.11}$$

Figure 2

- Equation(9.11) guarantees that each observation will be on the correct side of the hyperplane, provided that M is positive
- Under equation (9.10), the perpendicular distance from the ith observation to the hyperplane is given by

$$y_i(\beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip})$$

- M represents the margin of the hyperplane

Non-separable Case

- What if no separating hyperplane exists? A common scenario
- In other words, optimization problem (9.9-9.11) has no solution for $M > 0$
- A fix: develop a hyperplane that *almost* separates the classes, using a so-called *soft margin*
- Support vector classifier (a.k.a. soft margin classifier): the generalization of the maximal margin classifier to the non-separable case
- The margin is *soft* because it can be violated by some of the training observations

- Even if a separating hyperplane does exist, there are instances in which a classifier based on a separating hyperplane might not be desirable

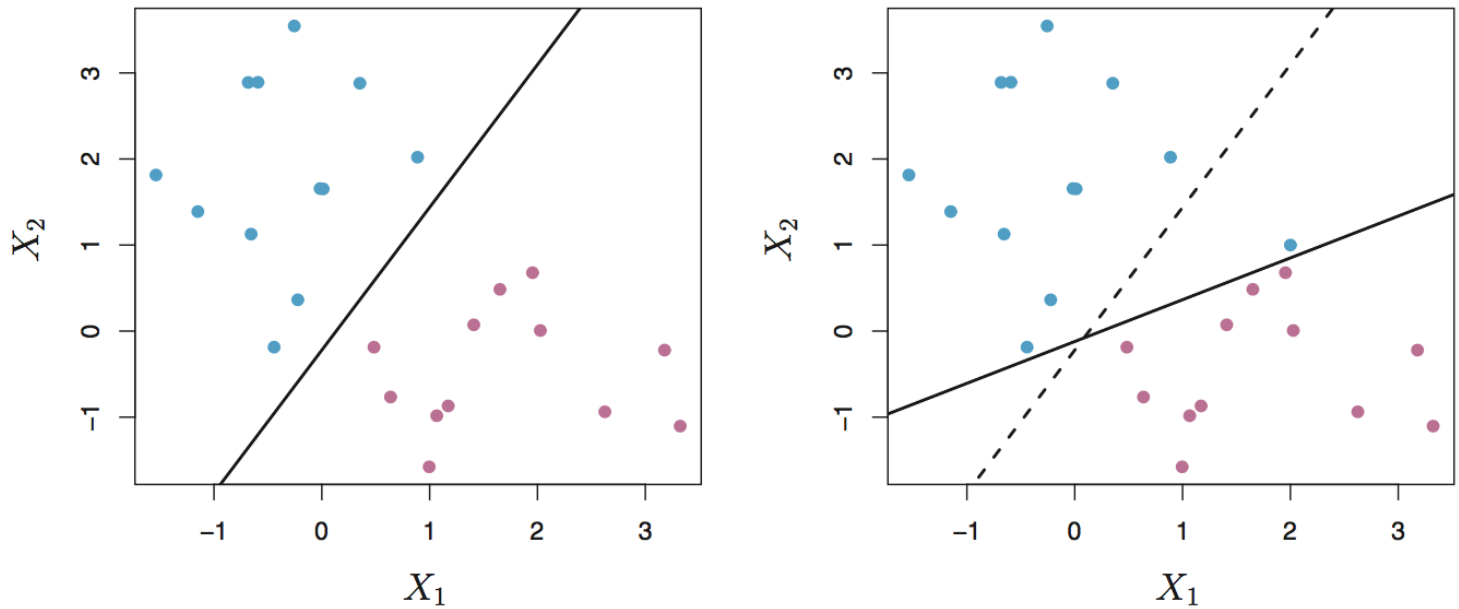


FIGURE 9.5. Left: *Two classes of observations are shown in blue and in purple, along with the maximal margin hyperplane.* Right: *An additional blue observation has been added, leading to a dramatic shift in the maximal margin hyperplane shown as a solid line. The dashed line indicates the maximal margin hyperplane that was obtained in the absence of this additional point.*

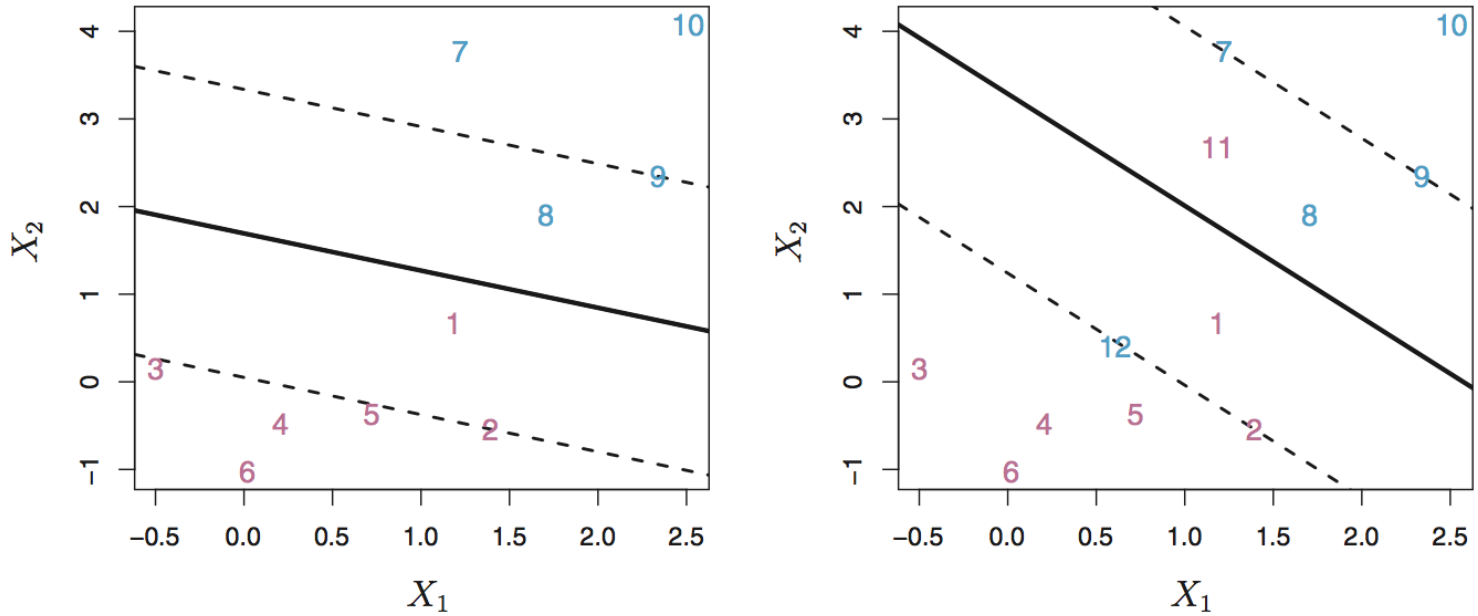


FIGURE 9.6. Left: *A support vector classifier was fit to a small data set. The hyperplane is shown as a solid line and the margins are shown as dashed lines.* Purple observations: *Observations* $3, 4, 5$, *and* 6 *are on the correct side of the margin, observation* 2 *is on the margin, and observation 1 is on the wrong side of the margin.* Blue observations: *Observations* 7 *and* 10 *are on the correct side of the margin, observation* 9 *is on the margin, and observation* 8 *is on the wrong side of the margin. No observations are on the wrong side of the hyperplane.* Right: *Same as left panel with two additional points,* 11 *and* 12. *These two observations are on the wrong side of the hyperplane and the wrong side of the margin.*

Figure 3

Optimization Program for Support Vector Classifier

$$\underset{\beta_0,\beta_1,\ldots,\beta_p,\epsilon_1,\ldots,\epsilon_n,M}{\text{maximize}} \; M \tag{9.12}$$

$$\text{subject to} \; \sum_{j=1}^{p} \beta_j^2 = 1, \tag{9.13}$$

$$y_i(\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \ldots + \beta_p x_{ip}) \geq M(1 - \epsilon_i), \tag{9.14}$$

$$\epsilon_i \geq 0, \; \sum_{i=1}^{n} \epsilon_i \leq C, \tag{9.15}$$

Figure 4

- C is a nonnegative tuning parameter; We can think of C as a budget for the amount that the margin can be violated by the n observations
- Q: as C increases, will the margin widen? How about the bias-variance trade-off?
- $\epsilon_1, \cdots, \epsilon_n$ are slack variables that allow individual observations to be on the wrong side of the margin or the hyperplane
- Once we solve (9.12 – 9.15), we classify a test point x^* as before
- Q: what does it mean for some ϵ_i to be positive or bigger than 1?

Classification with Non-linear Decision Boundaries

- Sometimes no linear decision boundary does well (recall a few cases)
- How to adapt the support vector classifiers to accommodate these cases?
- One solution is to introduce interaction terms, higher-order terms as new features, as we did for linear regression
- But this approach is often ad-hoc and incurs heavy computation burden if we introduce too many new features
- support vector machine (SVM): an extension of the support vector classifier that results from enlarging the feature space using kernels
- The detail is beyond the scope of the course, but we can take a look at some common kernels
- Interested readers can refer to Prof. Andrew Ng's notes: http://cs229.stanford.edu/notes/cs229-notes3.pdf
- Kernel: function that quantifies the similarity of two observations

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

- Other kernels

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

$$\text{radial kernel: } K(x_i, x_{i'}) = \exp\left(-\gamma \sum_{j=1}^{p} (x_{ij} - x_{i'j})^2\right)$$

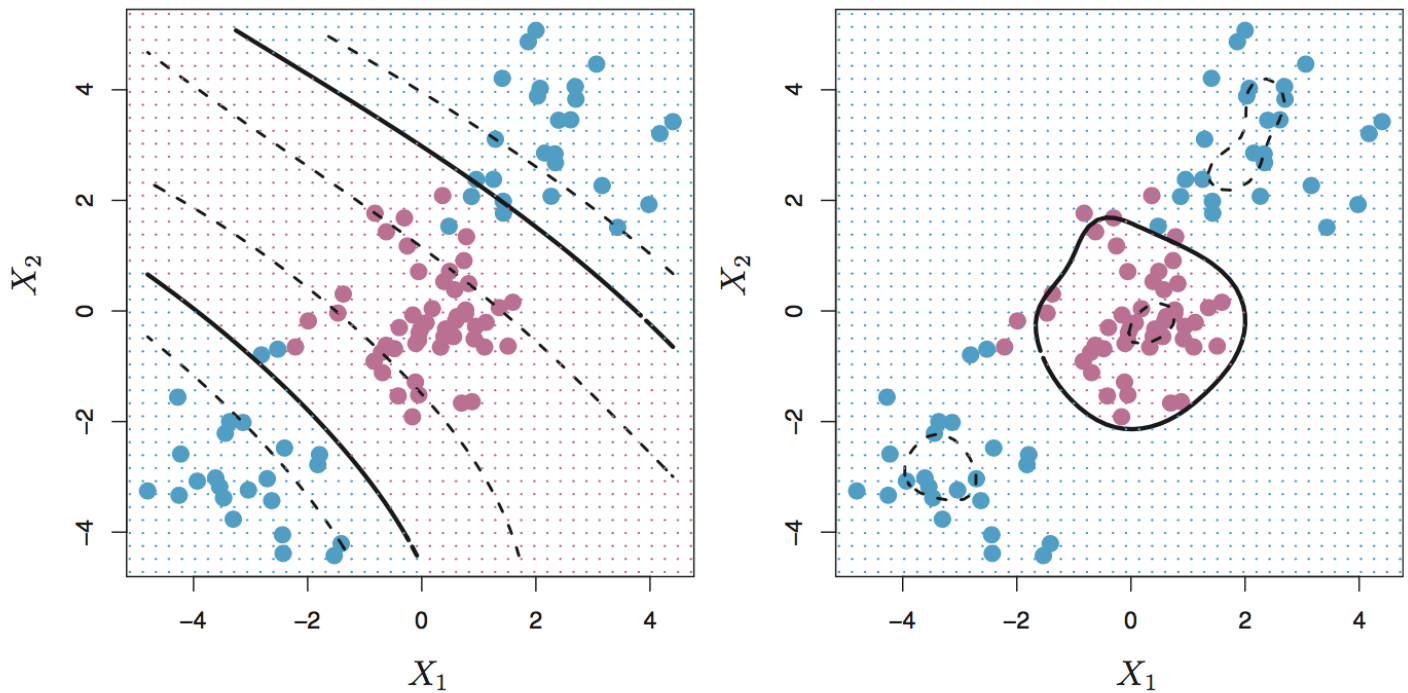


FIGURE 9.9. Left: *An SVM with a polynomial kernel of degree 3 is applied to the non-linear data from Figure 9.8, resulting in a far more appropriate decision rule.* Right: *An SVM with a radial kernel is applied. In this example, either kernel is capable of capturing the decision boundary.*