

5

Resampling Methods

Resampling methods are an indispensable tool in modern statistics. They involve repeatedly drawing samples from a training set and refitting a model of interest on each sample in order to obtain additional information about the fitted model. For example, in order to estimate the variability of a linear regression fit, we can repeatedly draw different samples from the training data, fit a linear regression to each new sample, and then examine the extent to which the resulting fits differ. Such an approach may allow us to obtain information that would not be available from fitting the model only once using the original training sample.

Resampling approaches can be computationally expensive, because they involve fitting the same statistical method multiple times using different subsets of the training data. However, due to recent advances in computing power, the computational requirements of resampling methods generally are not prohibitive. In this chapter, we discuss two of the most commonly used resampling methods, *cross-validation* and the *bootstrap*. Both methods are important tools in the practical application of many statistical learning procedures. For example, cross-validation can be used to estimate the test error associated with a given statistical learning method in order to evaluate its performance, or to select the appropriate level of flexibility. The process of evaluating a model's performance is known as *model assessment*, whereas the process of selecting the proper level of flexibility for a model is known as *model selection*. The bootstrap is used in several contexts, most commonly to provide a measure of accuracy of a parameter estimate or of a given statistical learning method.

model
assessment

model
selection

5.1 Cross-Validation

In Chapter 2 we discuss the distinction between the *test error rate* and the *training error rate*. The test error is the average error that results from using a statistical learning method to predict the response on a new observation—that is, a measurement that was not used in training the method. Given a data set, the use of a particular statistical learning method is warranted if it results in a low test error. The test error can be easily calculated if a designated test set is available. Unfortunately, this is usually not the case. In contrast, the training error can be easily calculated by applying the statistical learning method to the observations used in its training. But as we saw in Chapter 2, the training error rate often is quite different from the test error rate, and in particular the former can dramatically underestimate the latter.

In the absence of a very large designated test set that can be used to directly estimate the test error rate, a number of techniques can be used to estimate this quantity using the available training data. Some methods make a mathematical adjustment to the training error rate in order to estimate the test error rate. Such approaches are discussed in Chapter 6. In this section, we instead consider a class of methods that estimate the test error rate by *holding out* a subset of the training observations from the *fitting process*, and then applying the statistical learning method to those held out observations.

In Sections 5.1.1–5.1.4, for simplicity we assume that we are interested in performing regression with a quantitative response. In Section 5.1.5 we consider the case of classification with a qualitative response. As we will see, the key concepts remain the same regardless of whether the response is quantitative or qualitative.

5.1.1 The Validation Set Approach

Suppose that we would like to estimate the test error associated with fitting a particular statistical learning method on a set of observations. The *validation set approach*, displayed in Figure 5.1, is a very simple strategy for this task. It involves randomly dividing the available set of observations into two parts, a *training set* and a *validation set* or *hold-out set*. The model is fit on the training set, and the fitted model is used to predict the responses for the observations in the validation set. The resulting validation set error rate—typically assessed using MSE in the case of a quantitative response—provides an estimate of the test error rate.

validation
set approach

validation
set
hold-out set

We illustrate the validation set approach on the *Auto* data set. Recall from Chapter 3 that there appears to be a non-linear relationship between *mpg* and *horsepower*, and that a model that predicts *mpg* using *horsepower* and *horsepower*² gives better results than a model that uses only a linear term. It is natural to wonder whether a cubic or higher-order fit might provide



FIGURE 5.1. A schematic display of the validation set approach. A set of n observations are randomly split into a training set (shown in blue, containing observations 7, 22, and 13, among others) and a validation set (shown in beige, and containing observation 91, among others). The statistical learning method is fit on the training set, and its performance is evaluated on the validation set.

even better results. We answer this question in Chapter 3 by looking at the p -values associated with a cubic term and higher-order polynomial terms in a linear regression. But we could also answer this question using the validation method. We randomly split the 392 observations into two sets, a training set containing 196 of the data points, and a validation set containing the remaining 196 observations. The validation set error rates that result from fitting various regression models on the training sample and evaluating their performance on the validation sample, using MSE as a measure of validation set error, are shown in the left-hand panel of Figure 5.2. The validation set MSE for the quadratic fit is considerably smaller than for the linear fit. However, the validation set MSE for the cubic fit is actually slightly larger than for the quadratic fit. This implies that including a cubic term in the regression does not lead to better prediction than simply using a quadratic term.

Recall that in order to create the left-hand panel of Figure 5.2, we randomly divided the data set into two parts, a training set and a validation set. If we repeat the process of randomly splitting the sample set into two parts, we will get a somewhat different estimate for the test MSE. As an illustration, the right-hand panel of Figure 5.2 displays ten different validation set MSE curves from the `Auto` data set, produced using ten different random splits of the observations into training and validation sets. All ten curves indicate that the model with a quadratic term has a dramatically smaller validation set MSE than the model with only a linear term. Furthermore, all ten curves indicate that there is not much benefit in including cubic or higher-order polynomial terms in the model. But it is worth noting that each of the ten curves results in a different test MSE estimate for each of the ten regression models considered. And there is no consensus among the curves as to which model results in the smallest validation set MSE. Based on the variability among these curves, all that we can conclude with any confidence is that the linear fit is not adequate for this data.

The validation set approach is conceptually simple and is easy to implement. But it has two potential drawbacks:

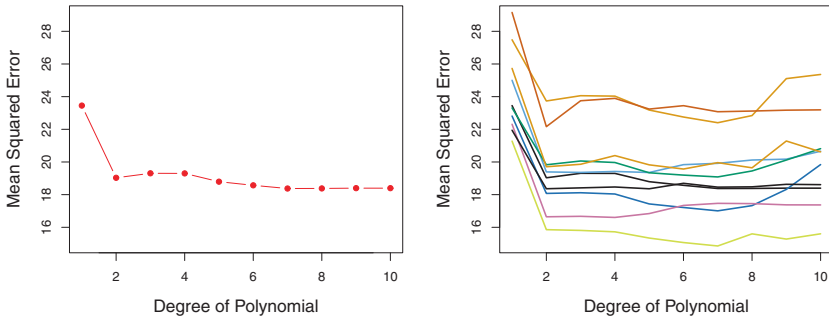


FIGURE 5.2. The validation set approach was used on the `Auto` data set in order to estimate the test error that results from predicting `mpg` using polynomial functions of `horsepower`. Left: Validation error estimates for a single split into training and validation data sets. Right: The validation method was repeated ten times, each time using a different random split of the observations into a training set and a validation set. This illustrates the variability in the estimated test MSE that results from this approach.

1. As is shown in the right-hand panel of Figure 5.2, the validation estimate of the test error rate can be highly variable, depending on precisely which observations are included in the training set and which observations are included in the validation set.
2. In the validation approach, only a subset of the observations—those that are included in the training set rather than in the validation set—are used to fit the model. Since statistical methods tend to perform worse when trained on fewer observations, this suggests that the validation set error rate may tend to overestimate the test error rate for the model fit on the entire data set.

In the coming subsections, we will present *cross-validation*, a refinement of the validation set approach that addresses these two issues.

5.1.2 Leave-One-Out Cross-Validation

Leave-one-out cross-validation (LOOCV) is closely related to the validation set approach of Section 5.1.1, but it attempts to address that method's drawbacks.

leave-one-out
cross-validation

Like the validation set approach, LOOCV involves splitting the set of observations into two parts. However, instead of creating two subsets of comparable size, a single observation (x_1, y_1) is used for the validation set, and the remaining observations $\{(x_2, y_2), \dots, (x_n, y_n)\}$ make up the training set. The statistical learning method is fit on the $n - 1$ training observations, and a prediction \hat{y}_1 is made for the excluded observation, using its value x_1 . Since (x_1, y_1) was not used in the fitting process, $\text{MSE}_1 =$

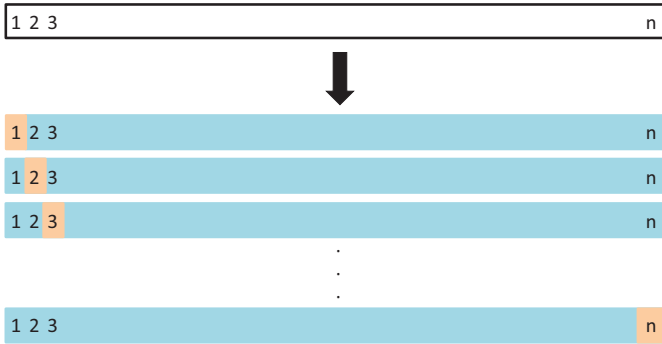


FIGURE 5.3. A schematic display of LOOCV. A set of n data points is repeatedly split into a training set (shown in blue) containing all but one observation, and a validation set that contains only that observation (shown in beige). The test error is then estimated by averaging the n resulting MSE's. The first training set contains all but observation 1, the second training set contains all but observation 2, and so forth.

$(y_1 - \hat{y}_1)^2$ provides an approximately unbiased estimate for the test error. But even though MSE_1 is unbiased for the test error, it is a poor estimate because it is highly variable, since it is based upon a single observation (x_1, y_1) .

We can repeat the procedure by selecting (x_2, y_2) for the validation data, training the statistical learning procedure on the $n - 1$ observations $\{(x_1, y_1), (x_3, y_3), \dots, (x_n, y_n)\}$, and computing $\text{MSE}_2 = (y_2 - \hat{y}_2)^2$. Repeating this approach n times produces n squared errors, $\text{MSE}_1, \dots, \text{MSE}_n$. The LOOCV estimate for the test MSE is the average of these n test error estimates:

$$\text{CV}_{(n)} = \frac{1}{n} \sum_{i=1}^n \text{MSE}_i. \quad (5.1)$$

A schematic of the LOOCV approach is illustrated in Figure 5.3.

LOOCV has a couple of major advantages over the validation set approach. First, it has far less bias. In LOOCV, we repeatedly fit the statistical learning method using training sets that contain $n - 1$ observations, almost as many as are in the entire data set. This is in contrast to the validation set approach, in which the training set is typically around half the size of the original data set. Consequently, the LOOCV approach tends not to overestimate the test error rate as much as the validation set approach does. Second, in contrast to the validation approach which will yield different results when applied repeatedly due to randomness in the training/validation set splits, performing LOOCV multiple times will

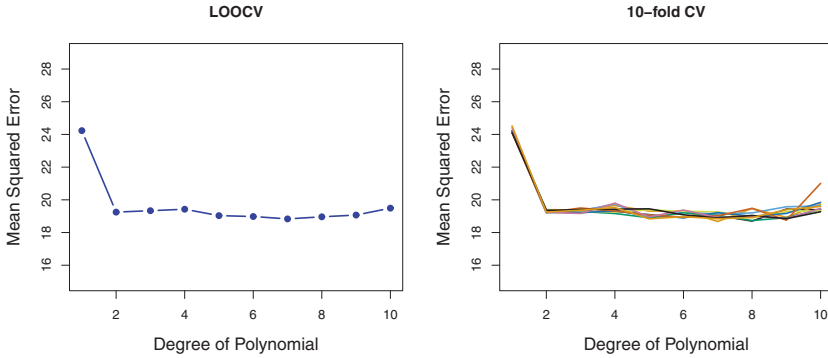


FIGURE 5.4. Cross-validation was used on the **Auto** data set in order to estimate the test error that results from predicting **mpg** using polynomial functions of **horsepower**. Left: The LOOCV error curve. Right: 10-fold CV was run nine separate times, each with a different random split of the data into ten parts. The figure shows the nine slightly different CV error curves.

always yield the same results: there is no randomness in the training/validation set splits.

We used LOOCV on the **Auto** data set in order to obtain an estimate of the test set MSE that results from fitting a linear regression model to predict **mpg** using polynomial functions of **horsepower**. The results are shown in the left-hand panel of Figure 5.4.

LOOCV has the potential to be expensive to implement, since the model has to be fit n times. This can be very time consuming if n is large, and if each individual model is slow to fit. With least squares linear or polynomial regression, an amazing shortcut makes the cost of LOOCV the same as that of a single model fit! The following formula holds:

$$CV_{(n)} = \frac{1}{n} \sum_{i=1}^n \left(\frac{y_i - \hat{y}_i}{1 - h_i} \right)^2, \quad (5.2)$$

where \hat{y}_i is the i th fitted value from the original least squares fit, and h_i is the leverage defined in (3.37) on page 98. This is like the ordinary MSE, except the i th residual is divided by $1 - h_i$. The leverage lies between $1/n$ and 1, and reflects the amount that an observation influences its own fit. Hence the residuals for high-leverage points are inflated in this formula by exactly the right amount for this equality to hold.

LOOCV is a very general method, and can be used with any kind of predictive modeling. For example we could use it with logistic regression or linear discriminant analysis, or any of the methods discussed in later

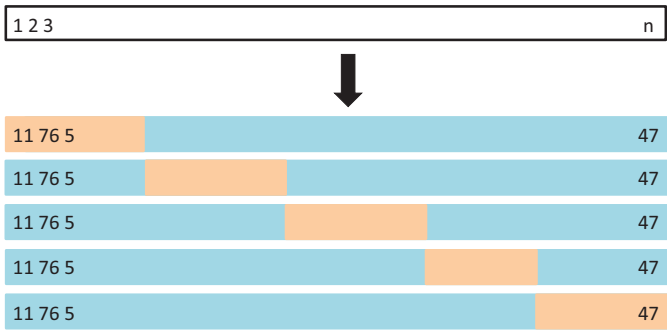


FIGURE 5.5. A schematic display of 5-fold CV. A set of n observations is randomly split into five non-overlapping groups. Each of these fifths acts as a validation set (shown in beige), and the remainder as a training set (shown in blue). The test error is estimated by averaging the five resulting MSE estimates.

chapters. The magic formula (5.2) does not hold in general, in which case the model has to be refit n times.

5.1.3 k -Fold Cross-Validation

An alternative to LOOCV is **k -fold CV**. This approach involves randomly dividing the set of observations into k groups, or *folds*, of approximately equal size. The first fold is treated as a validation set, and the method is fit on the remaining $k - 1$ folds. The mean squared error, MSE_1 , is then computed on the observations in the held-out fold. This procedure is repeated k times; each time, a different group of observations is treated as a validation set. This process results in k estimates of the test error, $\text{MSE}_1, \text{MSE}_2, \dots, \text{MSE}_k$. The k -fold CV estimate is computed by averaging these values,

$$\text{CV}_{(k)} = \frac{1}{k} \sum_{i=1}^k \text{MSE}_i. \quad (5.3)$$

Figure 5.5 illustrates the k -fold CV approach.

It is not hard to see that LOOCV is a special case of k -fold CV in which k is set to equal n . In practice, one typically performs k -fold CV using $k = 5$ or $k = 10$. What is the advantage of using $k = 5$ or $k = 10$ rather than $k = n$? The most obvious advantage is computational. LOOCV requires fitting the statistical learning method n times. This has the potential to be computationally expensive (except for linear models fit by least squares, in which case formula (5.2) can be used). But cross-validation is a very general approach that can be applied to almost any statistical learning method. Some statistical learning methods have computationally intensive fitting procedures, and so performing LOOCV may pose computational problems, especially if n is extremely large. In contrast, performing 10-fold

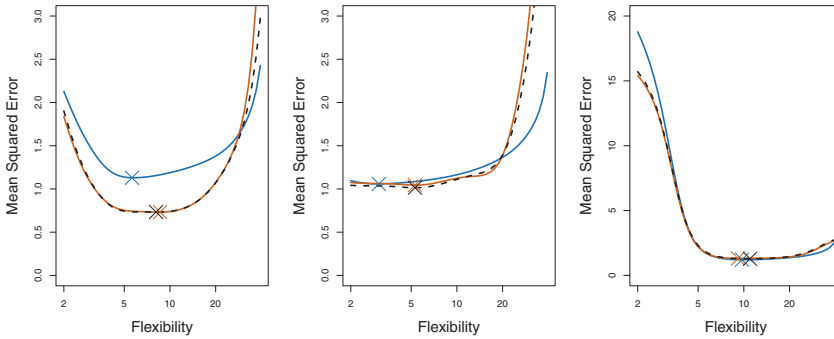


FIGURE 5.6. True and estimated test MSE for the simulated data sets in Figures 2.9 (left), 2.10 (center), and 2.11 (right). The true test MSE is shown in blue, the LOOCV estimate is shown as a black dashed line, and the 10-fold CV estimate is shown in orange. The crosses indicate the minimum of each of the MSE curves.

CV requires fitting the learning procedure only ten times, which may be much more feasible. As we see in Section 5.1.4, there also can be other non-computational advantages to performing 5-fold or 10-fold CV, which involve the bias-variance trade-off.

The right-hand panel of Figure 5.4 displays nine different 10-fold CV estimates for the `Auto` data set, each resulting from a different random split of the observations into ten folds. As we can see from the figure, there is some variability in the CV estimates as a result of the variability in how the observations are divided into ten folds. But this variability is typically much lower than the variability in the test error estimates that results from the validation set approach (right-hand panel of Figure 5.2).

When we examine real data, we do not know the *true* test MSE, and so it is difficult to determine the accuracy of the cross-validation estimate. However, if we examine simulated data, then we can compute the true test MSE, and can thereby evaluate the accuracy of our cross-validation results. In Figure 5.6, we plot the cross-validation estimates and true test error rates that result from applying smoothing splines to the simulated data sets illustrated in Figures 2.9–2.11 of Chapter 2. The true test MSE is displayed in blue. The black dashed and orange solid lines respectively show the estimated LOOCV and 10-fold CV estimates. In all three plots, the two cross-validation estimates are very similar. In the right-hand panel of Figure 5.6, the true test MSE and the cross-validation curves are almost identical. In the center panel of Figure 5.6, the two sets of curves are similar at the lower degrees of flexibility, while the CV curves overestimate the test set MSE for higher degrees of flexibility. In the left-hand panel of Figure 5.6, the CV curves have the correct general shape, but they underestimate the true test MSE.

When we perform cross-validation, our goal might be to determine how well a given statistical learning procedure can be expected to perform on independent data; in this case, the actual estimate of the test MSE is of interest. But at other times we are interested only in the location of the minimum point in the estimated test MSE curve. This is because we might be performing cross-validation on a number of statistical learning methods, or on a single method using different levels of flexibility, in order to identify the method that results in the lowest test error. For this purpose, the location of the minimum point in the estimated test MSE curve is important, but the actual value of the estimated test MSE is not. We find in Figure 5.6 that despite the fact that they sometimes underestimate the true test MSE, all of the CV curves come close to identifying the correct level of flexibility—that is, the flexibility level corresponding to the smallest test MSE.

5.1.4 Bias-Variance Trade-Off for k -Fold Cross-Validation

We mentioned in Section 5.1.3 that k -fold CV with $k < n$ has a computational advantage to LOOCV. But putting computational issues aside, a less obvious but potentially more important advantage of k -fold CV is that it often gives more accurate estimates of the test error rate than does LOOCV. This has to do with a bias-variance trade-off.

It was mentioned in Section 5.1.1 that the validation set approach can lead to overestimates of the test error rate, since in this approach the training set used to fit the statistical learning method contains only half the observations of the entire data set. Using this logic, it is not hard to see that LOOCV will give approximately unbiased estimates of the test error, since each training set contains $n - 1$ observations, which is almost as many as the number of observations in the full data set. And performing k -fold CV for, say, $k = 5$ or $k = 10$ will lead to an intermediate level of bias, since each training set contains $(k - 1)n/k$ observations—fewer than in the LOOCV approach, but substantially more than in the validation set approach. Therefore, from the perspective of bias reduction, it is clear that LOOCV is to be preferred to k -fold CV.

However, we know that bias is not the only source for concern in an estimating procedure; we must also consider the procedure's variance. It turns out that LOOCV has higher variance than does k -fold CV with $k < n$. Why is this the case? When we perform LOOCV, we are in effect averaging the outputs of n fitted models, each of which is trained on an almost identical set of observations; therefore, these outputs are highly (positively) correlated with each other. In contrast, when we perform k -fold CV with $k < n$, we are averaging the outputs of k fitted models that are somewhat less correlated with each other, since the overlap between the training sets in each model is smaller. Since the mean of many highly correlated quantities

has higher variance than does the mean of many quantities that are not as highly correlated, the test error estimate resulting from LOOCV tends to have higher variance than does the test error estimate resulting from k -fold CV.

To summarize, there is a bias-variance trade-off associated with the choice of k in k -fold cross-validation. Typically, given these considerations, one performs k -fold cross-validation using $k = 5$ or $k = 10$, as these values have been shown empirically to yield test error rate estimates that suffer neither from excessively high bias nor from very high variance.

5.1.5 Cross-Validation on Classification Problems

In this chapter so far, we have illustrated the use of cross-validation in the regression setting where the outcome Y is quantitative, and so have used MSE to quantify test error. But cross-validation can also be a very useful approach in the classification setting when Y is qualitative. In this setting, cross-validation works just as described earlier in this chapter, except that rather than using MSE to quantify test error, we instead use the number of misclassified observations. For instance, in the classification setting, the LOOCV error rate takes the form

$$\text{CV}_{(n)} = \frac{1}{n} \sum_{i=1}^n \text{Err}_i, \quad (5.4)$$

where $\text{Err}_i = I(y_i \neq \hat{y}_i)$. The k -fold CV error rate and validation set error rates are defined analogously.

As an example, we fit various logistic regression models on the two-dimensional classification data displayed in Figure 2.13. In the top-left panel of Figure 5.7, the black solid line shows the estimated decision boundary resulting from fitting a standard logistic regression model to this data set. Since this is simulated data, we can compute the *true* test error rate, which takes a value of 0.201 and so is substantially larger than the Bayes error rate of 0.133. Clearly logistic regression does not have enough flexibility to model the Bayes decision boundary in this setting. We can easily extend logistic regression to obtain a non-linear decision boundary by using polynomial functions of the predictors, as we did in the regression setting in Section 3.3.2. For example, we can fit a *quadratic* logistic regression model, given by

$$\log \left(\frac{p}{1-p} \right) = \beta_0 + \beta_1 X_1 + \beta_2 X_1^2 + \beta_3 X_2 + \beta_4 X_2^2. \quad (5.5)$$

The top-right panel of Figure 5.7 displays the resulting decision boundary, which is now curved. However, the test error rate has improved only slightly, to 0.197. A much larger improvement is apparent in the bottom-left panel

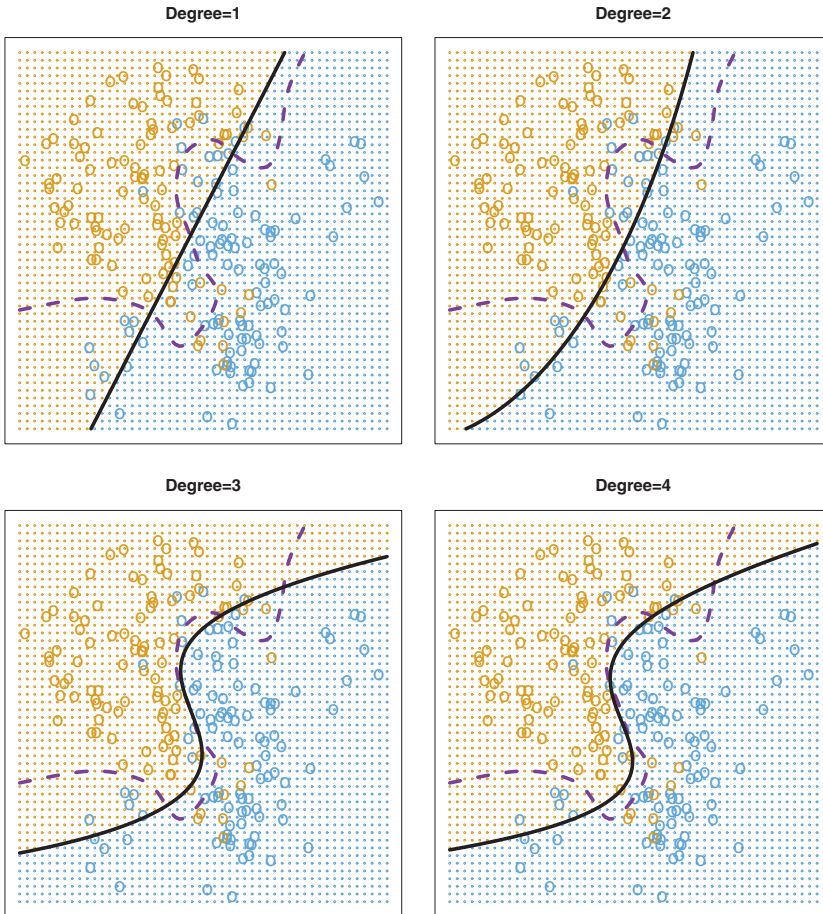


FIGURE 5.7. Logistic regression fits on the two-dimensional classification data displayed in Figure 2.13. The Bayes decision boundary is represented using a purple dashed line. Estimated decision boundaries from linear, quadratic, cubic and quartic (degrees 1–4) logistic regressions are displayed in black. The test error rates for the four logistic regression fits are respectively 0.201, 0.197, 0.160, and 0.162, while the Bayes error rate is 0.133.

of Figure 5.7, in which we have fit a logistic regression model involving cubic polynomials of the predictors. Now the test error rate has decreased to 0.160. Going to a quartic polynomial (bottom-right) slightly increases the test error.

In practice, for real data, the Bayes decision boundary and the test error rates are unknown. So how might we decide between the four logistic regression models displayed in Figure 5.7? We can use cross-validation in order to make this decision. The left-hand panel of Figure 5.8 displays in

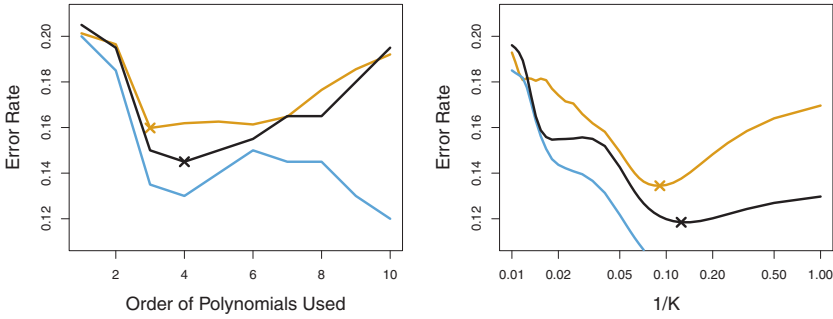


FIGURE 5.8. Test error (brown), training error (blue), and 10-fold CV error (black) on the two-dimensional classification data displayed in Figure 5.7. Left: Logistic regression using polynomial functions of the predictors. The order of the polynomials used is displayed on the x -axis. Right: The KNN classifier with different values of K , the number of neighbors used in the KNN classifier.

black the 10-fold CV error rates that result from fitting ten logistic regression models to the data, using polynomial functions of the predictors up to tenth order. The true test errors are shown in brown, and the training errors are shown in blue. As we have seen previously, the training error tends to decrease as the flexibility of the fit increases. (The figure indicates that though the training error rate doesn't quite decrease monotonically, it tends to decrease on the whole as the model complexity increases.) In contrast, the test error displays a characteristic U-shape. The 10-fold CV error rate provides a pretty good approximation to the test error rate. While it somewhat underestimates the error rate, it reaches a minimum when fourth-order polynomials are used, which is very close to the minimum of the test curve, which occurs when third-order polynomials are used. In fact, using fourth-order polynomials would likely lead to good test set performance, as the true test error rate is approximately the same for third, fourth, fifth, and sixth-order polynomials.

The right-hand panel of Figure 5.8 displays the same three curves using the KNN approach for classification, as a function of the value of K (which in this context indicates the number of neighbors used in the KNN classifier, rather than the number of CV folds used). Again the training error rate declines as the method becomes more flexible, and so we see that the training error rate cannot be used to select the optimal value for K . Though the cross-validation error curve slightly underestimates the test error rate, it takes on a minimum very close to the best value for K .