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An Introduction to Statistical Learning

with Applications in R

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2
Statistical Learning

2.1 What Is Statistical Learning?

In order to motivate our study of statistical learning, we begin with a simple example. Suppose that we are statistical consultants hired by a client to investigate the association between advertising and sales of a particular product. The `Advertising` data set consists of the `sales` of that product in 200 different markets, along with advertising budgets for the product in each of those markets for three different media: `TV`, `radio`, and `newspaper`. The data are displayed in Figure 2.1. It is not possible for our client to directly increase sales of the product. On the other hand, they can control the advertising expenditure in each of the three media. Therefore, if we determine that there is an association between advertising and sales, then we can instruct our client to adjust advertising budgets, thereby indirectly increasing sales. In other words, our goal is to develop an accurate model that can be used to predict sales on the basis of the three media budgets.

In this setting, the advertising budgets are *input variables* while `sales` is an *output variable*. The input variables are typically denoted using the symbol X, with a subscript to distinguish them. So X_1 might be the `TV` budget, X_2 the `radio` budget, and X_3 the `newspaper` budget. The inputs go by different names, such as *predictors*, *independent variables*, *features*, or sometimes just *variables*. The output variable—in this case, `sales`—is often called the *response* or *dependent variable*, and is typically denoted using the symbol Y. Throughout this book, we will use all of these terms interchangeably.

input variable
output variable
predictor
independent variable
feature
variable
response
dependent variable

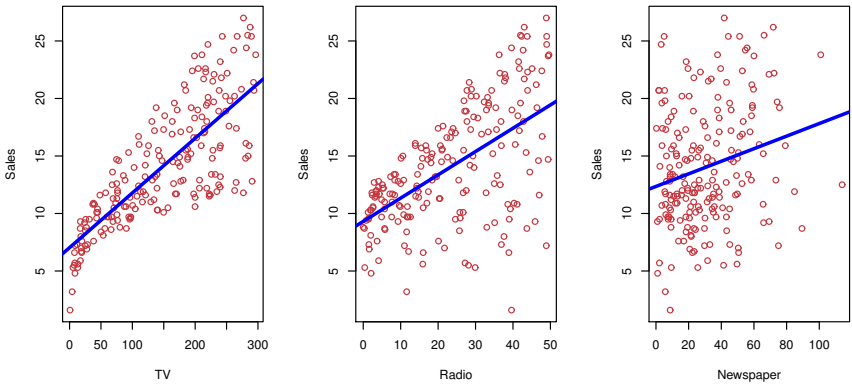


FIGURE 2.1. *The* `Advertising` *data set. The plot displays* `sales`*, in thousands of units, as a function of* `TV`*,* `radio`*, and* `newspaper` *budgets, in thousands of dollars, for* 200 *different markets. In each plot we show the simple least squares fit of* `sales` *to that variable, as described in Chapter 3. In other words, each blue line represents a simple model that can be used to predict* `sales` *using* `TV`*,* `radio`*, and* `newspaper`*, respectively.*

More generally, suppose that we observe a quantitative response Y and p different predictors, $X_1, X_2, \ldots, X_p$. We assume that there is some relationship between Y and $X = (X_1, X_2, \ldots, X_p)$, which can be written in the very general form

$$Y = f(X) + \epsilon. \tag{2.1}$$

Here f is some fixed but unknown function of $X_1, \ldots, X_p$, and ϵ is a random *error term*, which is independent of X and has mean zero. In this formulation, f represents the *systematic* information that X provides about Y.

error term

systematic

As another example, consider the left-hand panel of Figure 2.2, a plot of `income` versus `years of education` for 30 individuals in the `Income` data set. The plot suggests that one might be able to predict `income` using `years of education`. However, the function f that connects the input variable to the output variable is in general unknown. In this situation one must estimate f based on the observed points. Since `Income` is a simulated data set, f is known and is shown by the blue curve in the right-hand panel of Figure 2.2. The vertical lines represent the error terms ϵ. We note that some of the 30 observations lie above the blue curve and some lie below it; overall, the errors have approximately mean zero.

In general, the function f may involve more than one input variable. In Figure 2.3 we plot `income` as a function of `years of education` and `seniority`. Here f is a two-dimensional surface that must be estimated based on the observed data.

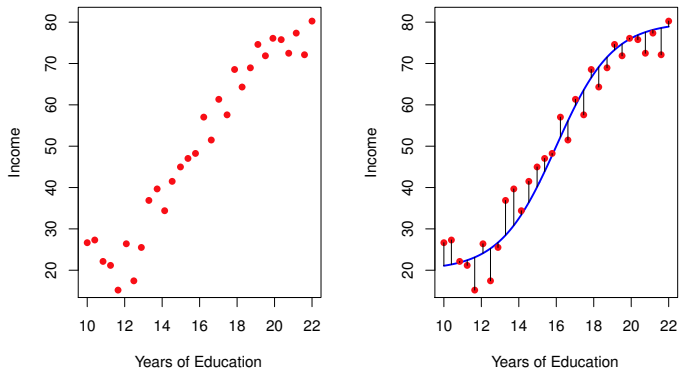


FIGURE 2.2. *The* Income *data set.* Left: *The red dots are the observed values of* income *(in thousands of dollars) and* years of education *for* 30 *individuals.* Right: *The blue curve represents the true underlying relationship between* income *and* years of education*, which is generally unknown (but is known in this case because the data were simulated). The black lines represent the error associated with each observation. Note that some errors are positive (if an observation lies above the blue curve) and some are negative (if an observation lies below the curve). Overall, these errors have approximately mean zero.*

In essence, statistical learning refers to a set of approaches for estimating f. In this chapter we outline some of the key theoretical concepts that arise in estimating f, as well as tools for evaluating the estimates obtained.

2.1.1 Why Estimate f?

There are two main reasons that we may wish to estimate f: *prediction* and *inference*. We discuss each in turn.

Prediction

In many situations, a set of inputs X are readily available, but the output Y cannot be easily obtained. In this setting, since the error term averages to zero, we can predict Y using

$$\hat{Y} = \hat{f}(X), \tag{2.2}$$

where $\hat{f}$ represents our estimate for f, and $\hat{Y}$ represents the resulting prediction for Y. In this setting, $\hat{f}$ is often treated as a *black box*, in the sense that one is not typically concerned with the exact form of $\hat{f}$, provided that it yields accurate predictions for Y.

As an example, suppose that $X_1, \ldots, X_p$ are characteristics of a patient's blood sample that can be easily measured in a lab, and Y is a variable encoding the patient's risk for a severe adverse reaction to a particular

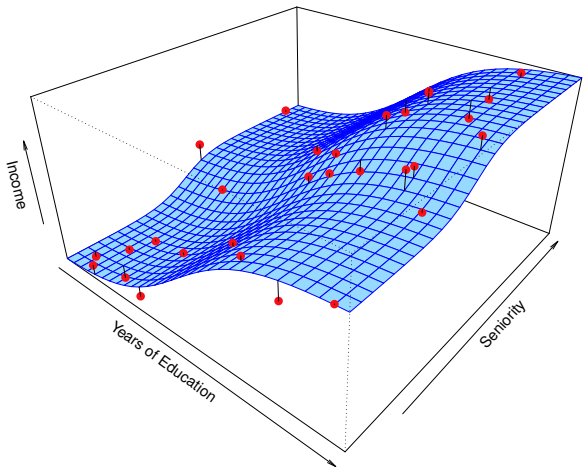


FIGURE 2.3. *The plot displays* `income` *as a function of* `years of education` *and* `seniority` *in the* `Income` *data set. The blue surface represents the true underlying relationship between* `income` *and* `years of education` *and* `seniority`*, which is known since the data are simulated. The red dots indicate the observed values of these quantities for* 30 *individuals.*

drug. It is natural to seek to predict Y using X, since we can then avoid giving the drug in question to patients who are at high risk of an adverse reaction—that is, patients for whom the estimate of Y is high.

The accuracy of $\hat{Y}$ as a prediction for Y depends on two quantities, which we will call the *reducible error* and the *irreducible error*. In general, $\hat{f}$ will not be a perfect estimate for f, and this inaccuracy will introduce some error. This error is *reducible* because we can potentially improve the accuracy of $\hat{f}$ by using the most appropriate statistical learning technique to estimate f. However, even if it were possible to form a perfect estimate for f, so that our estimated response took the form $\hat{Y} = f(X)$, our prediction would still have some error in it! This is because Y is also a function of ϵ, which, by definition, cannot be predicted using X. Therefore, variability associated with ϵ also affects the accuracy of our predictions. This is known as the *irreducible* error, because no matter how well we estimate f, we cannot reduce the error introduced by ϵ.

reducible error

irreducible error

Why is the irreducible error larger than zero? The quantity ϵ may contain unmeasured variables that are useful in predicting Y: since we don't measure them, f cannot use them for its prediction. The quantity ϵ may also contain unmeasurable variation. For example, the risk of an adverse reaction might vary for a given patient on a given day, depending on manufacturing variation in the drug itself or the patient's general feeling of well-being on that day.

Consider a given estimate $\hat{f}$ and a set of predictors X, which yields the prediction $\hat{Y} = \hat{f}(X)$. Assume for a moment that both $\hat{f}$ and X are fixed, so that the only variability comes from ϵ. Then, it is easy to show that

$$\begin{aligned} \mathrm{E}(Y - \hat{Y})^2 &= \mathrm{E}[f(X) + \epsilon - \hat{f}(X)]^2 \\ &= \underbrace{[f(X) - \hat{f}(X)]^2}_{\text{Reducible}} + \underbrace{\mathrm{Var}(\epsilon)}_{\text{Irreducible}}, \end{aligned} \tag{2.3}$$

where $\mathrm{E}(Y - \hat{Y})^2$ represents the average, or *expected value*, of the squared difference between the predicted and actual value of Y, and $\mathrm{Var}(\epsilon)$ represents the *variance* associated with the error term ϵ.

expected value

variance

The focus of this book is on techniques for estimating f with the aim of minimizing the reducible error. It is important to keep in mind that the irreducible error will always provide an upper bound on the accuracy of our prediction for Y. This bound is almost always unknown in practice.

Inference

We are often interested in understanding the association between Y and $X_1, \ldots, X_p$. In this situation we wish to estimate f, but our goal is not necessarily to make predictions for Y. Now $\hat{f}$ cannot be treated as a black box, because we need to know its exact form. In this setting, one may be interested in answering the following questions:

- *Which predictors are associated with the response?* It is often the case that only a small fraction of the available predictors are substantially associated with Y. Identifying the few *important* predictors among a large set of possible variables can be extremely useful, depending on the application.
- *What is the relationship between the response and each predictor?* Some predictors may have a positive relationship with Y, in the sense that larger values of the predictor are associated with larger values of Y. Other predictors may have the opposite relationship. Depending on the complexity of f, the relationship between the response and a given predictor may also depend on the values of the other predictors.
- *Can the relationship between Y and each predictor be adequately summarized using a linear equation, or is the relationship more complicated?* Historically, most methods for estimating f have taken a linear form. In some situations, such an assumption is reasonable or even desirable. But often the true relationship is more complicated, in which case a linear model may not provide an accurate representation of the relationship between the input and output variables.

In this book, we will see a number of examples that fall into the prediction setting, the inference setting, or a combination of the two.

For instance, consider a company that is interested in conducting a direct-marketing campaign. The goal is to identify individuals who are likely to respond positively to a mailing, based on observations of demographic variables measured on each individual. In this case, the demographic variables serve as predictors, and response to the marketing campaign (either positive or negative) serves as the outcome. The company is not interested in obtaining a deep understanding of the relationships between each individual predictor and the response; instead, the company simply wants to accurately predict the response using the predictors. This is an example of modeling for prediction.

In contrast, consider the `Advertising` data illustrated in Figure 2.1. One may be interested in answering questions such as:

- *Which media are associated with sales?*
- *Which media generate the biggest boost in sales?* or
- *How large of an increase in sales is associated with a given increase in TV advertising?*

This situation falls into the inference paradigm. Another example involves modeling the brand of a product that a customer might purchase based on variables such as price, store location, discount levels, competition price, and so forth. In this situation one might really be most interested in the association between each variable and the probability of purchase. For instance, *to what extent is the product's price associated with sales?* This is an example of modeling for inference.

Finally, some modeling could be conducted both for prediction and inference. For example, in a real estate setting, one may seek to relate values of homes to inputs such as crime rate, zoning, distance from a river, air quality, schools, income level of community, size of houses, and so forth. In this case one might be interested in the association between each individual input variable and housing price—for instance, *how much extra will a house be worth if it has a view of the river?* This is an inference problem. Alternatively, one may simply be interested in predicting the value of a home given its characteristics: *is this house under- or over-valued?* This is a prediction problem.

Depending on whether our ultimate goal is prediction, inference, or a combination of the two, different methods for estimating f may be appropriate. For example, *linear models* allow for relatively simple and interpretable inference, but may not yield as accurate predictions as some other approaches. In contrast, some of the highly non-linear approaches that we discuss in the later chapters of this book can potentially provide quite accurate predictions for Y, but this comes at the expense of a less interpretable model for which inference is more challenging.

linear model

2.1.2 How Do We Estimate f?

Throughout this book, we explore many linear and non-linear approaches for estimating f. However, these methods generally share certain characteristics. We provide an overview of these shared characteristics in this section. We will always assume that we have observed a set of n different data points. For example in Figure 2.2 we observed $n = 30$ data points. These observations are called the *training data* because we will use these observations to train, or teach, our method how to estimate f. Let x_{ij} represent the value of the jth predictor, or input, for observation i, where $i = 1, 2, \ldots, n$ and $j = 1, 2, \ldots, p$. Correspondingly, let y_i represent the response variable for the ith observation. Then our training data consist of $\{(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)\}$ where $x_i = (x_{i1}, x_{i2}, \ldots, x_{ip})^T$.

training data

Our goal is to apply a statistical learning method to the training data in order to estimate the unknown function f. In other words, we want to find a function $\hat{f}$ such that $Y \approx \hat{f}(X)$ for any observation (X, Y). Broadly speaking, most statistical learning methods for this task can be characterized as either *parametric* or *non-parametric*. We now briefly discuss these two types of approaches.

parametric
non-parametric

Parametric Methods

Parametric methods involve a two-step model-based approach.

1. First, we make an assumption about the functional form, or shape, of f. For example, one very simple assumption is that f is linear in X:

$$f(X) = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_p X_p. \tag{2.4}$$

   This is a *linear model*, which will be discussed extensively in Chapter 3. Once we have assumed that f is linear, the problem of estimating f is greatly simplified. Instead of having to estimate an entirely arbitrary p-dimensional function $f(X)$, one only needs to estimate the $p + 1$ coefficients $\beta_0, \beta_1, \ldots, \beta_p$.

2. After a model has been selected, we need a procedure that uses the training data to *fit* or *train* the model. In the case of the linear model (2.4), we need to estimate the parameters $\beta_0, \beta_1, \ldots, \beta_p$. That is, we want to find values of these parameters such that

fit
train

$$Y \approx \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_p X_p.$$

   The most common approach to fitting the model (2.4) is referred to as *(ordinary) least squares*, which we discuss in Chapter 3. However, least squares is one of many possible ways to fit the linear model. In Chapter 6, we discuss other approaches for estimating the parameters in (2.4).

least squares

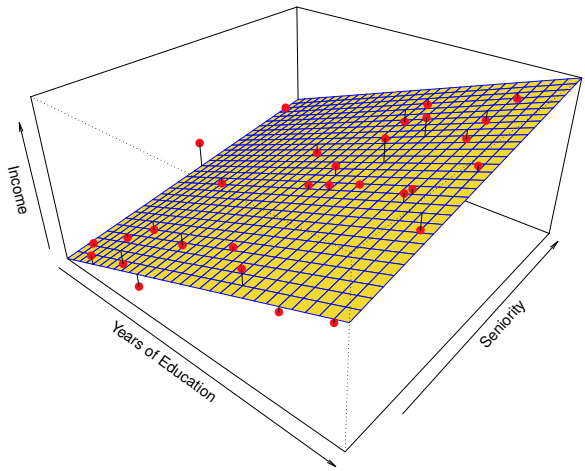


FIGURE 2.4. *A linear model fit by least squares to the* Income *data from Figure 2.3. The observations are shown in red, and the yellow plane indicates the least squares fit to the data.*

The model-based approach just described is referred to as *parametric*; it reduces the problem of estimating f down to one of estimating a set of parameters. Assuming a parametric form for f simplifies the problem of estimating f because it is generally much easier to estimate a set of parameters, such as $\beta_0, \beta_1, \ldots, \beta_p$ in the linear model (2.4), than it is to fit an entirely arbitrary function f. The potential disadvantage of a parametric approach is that the model we choose will usually not match the true unknown form of f. If the chosen model is too far from the true f, then our estimate will be poor. We can try to address this problem by choosing *flexible* models that can fit many different possible functional forms for f. But in general, fitting a more flexible model requires estimating a greater number of parameters. These more complex models can lead to a phenomenon known as *overfitting* the data, which essentially means they follow the errors, or *noise*, too closely. These issues are discussed throughout this book.

flexible

overfitting

noise

Figure 2.4 shows an example of the parametric approach applied to the Income data from Figure 2.3. We have fit a linear model of the form

$$\texttt{income} \approx \beta_0 + \beta_1 \times \texttt{education} + \beta_2 \times \texttt{seniority}.$$

Since we have assumed a linear relationship between the response and the two predictors, the entire fitting problem reduces to estimating β_0, β_1, and β_2, which we do using least squares linear regression. Comparing Figure 2.3 to Figure 2.4, we can see that the linear fit given in Figure 2.4 is not quite right: the true f has some curvature that is not captured in the linear fit. However, the linear fit still appears to do a reasonable job of capturing the

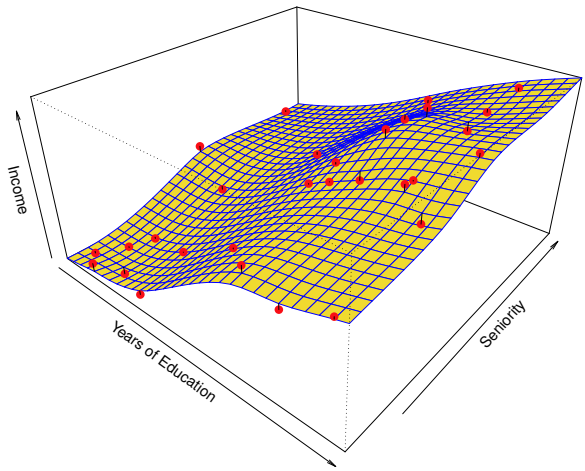


FIGURE 2.5. *A smooth thin-plate spline fit to the* `Income` *data from Figure 2.3 is shown in yellow; the observations are displayed in red. Splines are discussed in Chapter 7.*

positive relationship between `years of education` and `income`, as well as the slightly less positive relationship between `seniority` and `income`. It may be that with such a small number of observations, this is the best we can do.

Non-Parametric Methods

Non-parametric methods do not make explicit assumptions about the functional form of f. Instead they seek an estimate of f that gets as close to the data points as possible without being too rough or wiggly. Such approaches can have a major advantage over parametric approaches: by avoiding the assumption of a particular functional form for f, they have the potential to accurately fit a wider range of possible shapes for f. Any parametric approach brings with it the possibility that the functional form used to estimate f is very different from the true f, in which case the resulting model will not fit the data well. In contrast, non-parametric approaches completely avoid this danger, since essentially no assumption about the form of f is made. But non-parametric approaches do suffer from a major disadvantage: since they do not reduce the problem of estimating f to a small number of parameters, a very large number of observations (far more than is typically needed for a parametric approach) is required in order to obtain an accurate estimate for f.

An example of a non-parametric approach to fitting the `Income` data is shown in Figure 2.5. A *thin-plate spline* is used to estimate f. This approach does not impose any pre-specified model on f. It instead attempts to produce an estimate for f that is as close as possible to the observed data, subject to the fit—that is, the yellow surface in Figure 2.5—being

thin-plate spline

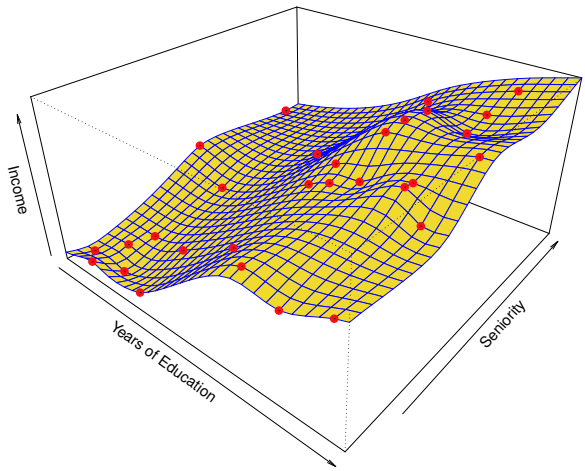


FIGURE 2.6. *A rough thin-plate spline fit to the* `Income` *data from Figure 2.3. This fit makes zero errors on the training data.*

smooth. In this case, the non-parametric fit has produced a remarkably accurate estimate of the true f shown in Figure 2.3. In order to fit a thin-plate spline, the data analyst must select a level of smoothness. Figure 2.6 shows the same thin-plate spline fit using a lower level of smoothness, allowing for a rougher fit. The resulting estimate fits the observed data perfectly! However, the spline fit shown in Figure 2.6 is far more variable than the true function f, from Figure 2.3. This is an example of overfitting the data, which we discussed previously. It is an undesirable situation because the fit obtained will not yield accurate estimates of the response on new observations that were not part of the original training data set. We discuss methods for choosing the *correct* amount of smoothness in Chapter 5. Splines are discussed in Chapter 7.

As we have seen, there are advantages and disadvantages to parametric and non-parametric methods for statistical learning. We explore both types of methods throughout this book.

2.1.3 The Trade-Off Between Prediction Accuracy and Model Interpretability

Of the many methods that we examine in this book, some are less flexible, or more restrictive, in the sense that they can produce just a relatively small range of shapes to estimate f. For example, linear regression is a relatively inflexible approach, because it can only generate linear functions such as the lines shown in Figure 2.1 or the plane shown in Figure 2.4. Other methods, such as the thin plate splines shown in Figures 2.5 and 2.6,

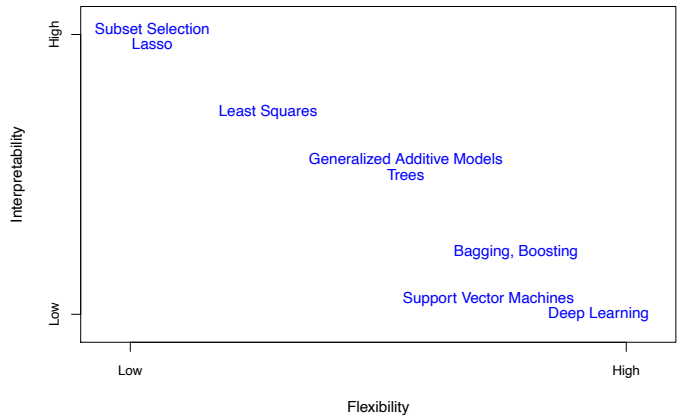


FIGURE 2.7. *A representation of the tradeoff between flexibility and interpretability, using different statistical learning methods. In general, as the flexibility of a method increases, its interpretability decreases.*

are considerably more flexible because they can generate a much wider range of possible shapes to estimate f.

One might reasonably ask the following question: *why would we ever choose to use a more restrictive method instead of a very flexible approach?* There are several reasons that we might prefer a more restrictive model. If we are mainly interested in inference, then restrictive models are much more interpretable. For instance, when inference is the goal, the linear model may be a good choice since it will be quite easy to understand the relationship between Y and $X_1, X_2, \ldots, X_p$. In contrast, very flexible approaches, such as the splines discussed in Chapter 7 and displayed in Figures 2.5 and 2.6, and the boosting methods discussed in Chapter 8, can lead to such complicated estimates of f that it is difficult to understand how any individual predictor is associated with the response.

Figure 2.7 provides an illustration of the trade-off between flexibility and interpretability for some of the methods that we cover in this book. Least squares linear regression, discussed in Chapter 3, is relatively inflexible but is quite interpretable. The *lasso*, discussed in Chapter 6, relies upon the linear model (2.4) but uses an alternative fitting procedure for estimating the coefficients $\beta_0, \beta_1, \ldots, \beta_p$. The new procedure is more restrictive in estimating the coefficients, and sets a number of them to exactly zero. Hence in this sense the lasso is a less flexible approach than linear regression. It is also more interpretable than linear regression, because in the final model the response variable will only be related to a small subset of the predictors—namely, those with nonzero coefficient estimates. *Generalized additive models* (GAMs), discussed in Chapter 7, instead extend the linear model (2.4) to allow for certain non-linear relationships. Consequently,

lasso

generalized additive model

GAMs are more flexible than linear regression. They are also somewhat less interpretable than linear regression, because the relationship between each predictor and the response is now modeled using a curve. Finally, fully non-linear methods such as *bagging*, *boosting*, *support vector machines* with non-linear kernels, and *neural networks* (deep learning), discussed in Chapters 8, 9, and 10, are highly flexible approaches that are harder to interpret.

bagging
boosting
support vector machine

We have established that when inference is the goal, there are clear advantages to using simple and relatively inflexible statistical learning methods. In some settings, however, we are only interested in prediction, and the interpretability of the predictive model is simply not of interest. For instance, if we seek to develop an algorithm to predict the price of a stock, our sole requirement for the algorithm is that it predict accurately—interpretability is not a concern. In this setting, we might expect that it will be best to use the most flexible model available. Surprisingly, this is not always the case! We will often obtain more accurate predictions using a less flexible method. This phenomenon, which may seem counterintuitive at first glance, has to do with the potential for overfitting in highly flexible methods. We saw an example of overfitting in Figure 2.6. We will discuss this very important concept further in Section 2.2 and throughout this book.

2.1.4 Supervised Versus Unsupervised Learning

Most statistical learning problems fall into one of two categories: *supervised* or *unsupervised*. The examples that we have discussed so far in this chapter all fall into the supervised learning domain. For each observation of the predictor measurement(s) x_i, $i = 1, \ldots, n$ there is an associated response measurement y_i. We wish to fit a model that relates the response to the predictors, with the aim of accurately predicting the response for future observations (prediction) or better understanding the relationship between the response and the predictors (inference). Many classical statistical learning methods such as linear regression and *logistic regression* (Chapter 4), as well as more modern approaches such as GAM, boosting, and support vector machines, operate in the supervised learning domain. The vast majority of this book is devoted to this setting.

supervised
unsupervised
logistic regression

By contrast, unsupervised learning describes the somewhat more challenging situation in which for every observation $i = 1, \ldots, n$, we observe a vector of measurements x_i but no associated response y_i. It is not possible to fit a linear regression model, since there is no response variable to predict. In this setting, we are in some sense working blind; the situation is referred to as *unsupervised* because we lack a response variable that can supervise our analysis. What sort of statistical analysis is possible? We can seek to understand the relationships between the variables or between the observations. One statistical learning tool that we may use

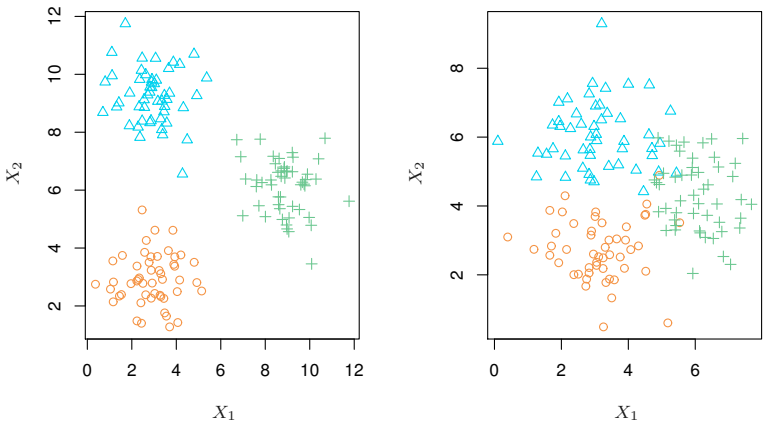


FIGURE 2.8. *A clustering data set involving three groups. Each group is shown using a different colored symbol.* Left: *The three groups are well-separated. In this setting, a clustering approach should successfully identify the three groups.* Right: *There is some overlap among the groups. Now the clustering task is more challenging.*

in this setting is *cluster analysis*, or clustering. The goal of cluster analysis is to ascertain, on the basis of $x_1, \ldots, x_n$, whether the observations fall into relatively distinct groups. For example, in a market segmentation study we might observe multiple characteristics (variables) for potential customers, such as zip code, family income, and shopping habits. We might believe that the customers fall into different groups, such as big spenders versus low spenders. If the information about each customer's spending patterns were available, then a supervised analysis would be possible. However, this information is not available—that is, we do not know whether each potential customer is a big spender or not. In this setting, we can try to cluster the customers on the basis of the variables measured, in order to identify distinct groups of potential customers. Identifying such groups can be of interest because it might be that the groups differ with respect to some property of interest, such as spending habits.

cluster analysis

Figure 2.8 provides a simple illustration of the clustering problem. We have plotted 150 observations with measurements on two variables, X_1 and X_2. Each observation corresponds to one of three distinct groups. For illustrative purposes, we have plotted the members of each group using different colors and symbols. However, in practice the group memberships are unknown, and the goal is to determine the group to which each observation belongs. In the left-hand panel of Figure 2.8, this is a relatively easy task because the groups are well-separated. By contrast, the right-hand panel illustrates a more challenging setting in which there is some overlap

between the groups. A clustering method could not be expected to assign all of the overlapping points to their correct group (blue, green, or orange).

In the examples shown in Figure 2.8, there are only two variables, and so one can simply visually inspect the scatterplots of the observations in order to identify clusters. However, in practice, we often encounter data sets that contain many more than two variables. In this case, we cannot easily plot the observations. For instance, if there are p variables in our data set, then $p(p-1)/2$ distinct scatterplots can be made, and visual inspection is simply not a viable way to identify clusters. For this reason, automated clustering methods are important. We discuss clustering and other unsupervised learning approaches in Chapter 12.

Many problems fall naturally into the supervised or unsupervised learning paradigms. However, sometimes the question of whether an analysis should be considered supervised or unsupervised is less clear-cut. For instance, suppose that we have a set of n observations. For m of the observations, where $m < n$, we have both predictor measurements and a response measurement. For the remaining $n - m$ observations, we have predictor measurements but no response measurement. Such a scenario can arise if the predictors can be measured relatively cheaply but the corresponding responses are much more expensive to collect. We refer to this setting as a *semi-supervised learning* problem. In this setting, we wish to use a statistical learning method that can incorporate the m observations for which response measurements are available as well as the $n - m$ observations for which they are not. Although this is an interesting topic, it is beyond the scope of this book.

semi-supervised learning

2.1.5 Regression Versus Classification Problems

Variables can be characterized as either *quantitative* or *qualitative* (also known as *categorical*). Quantitative variables take on numerical values. Examples include a person's age, height, or income, the value of a house, and the price of a stock. In contrast, qualitative variables take on values in one of K different *classes*, or categories. Examples of qualitative variables include a person's marital status (married or not), the brand of product purchased (brand A, B, or C), whether a person defaults on a debt (yes or no), or a cancer diagnosis (Acute Myelogenous Leukemia, Acute Lymphoblastic Leukemia, or No Leukemia). We tend to refer to problems with a quantitative response as *regression* problems, while those involving a qualitative response are often referred to as *classification* problems. However, the distinction is not always that crisp. Least squares linear regression (Chapter 3) is used with a quantitative response, whereas logistic regression (Chapter 4) is typically used with a qualitative (two-class, or *binary*) response. Thus, despite its name, logistic regression is a classification method. But since it estimates class probabilities, it can be thought of as a regression method as well. Some statistical methods, such as K-nearest neighbors

quantitative
qualitative
categorical

class

regression
classification

binary

(Chapters 2 and 4) and boosting (Chapter 8), can be used in the case of either quantitative or qualitative responses.

We tend to select statistical learning methods on the basis of whether the response is quantitative or qualitative; i.e. we might use linear regression when quantitative and logistic regression when qualitative. However, whether the *predictors* are qualitative or quantitative is generally considered less important. Most of the statistical learning methods discussed in this book can be applied regardless of the predictor variable type, provided that any qualitative predictors are properly *coded* before the analysis is performed. This is discussed in Chapter 3.

2.2 Assessing Model Accuracy

One of the key aims of this book is to introduce the reader to a wide range of statistical learning methods that extend far beyond the standard linear regression approach. Why is it necessary to introduce so many different statistical learning approaches, rather than just a single *best* method? *There is no free lunch in statistics:* no one method dominates all others over all possible data sets. On a particular data set, one specific method may work best, but some other method may work better on a similar but different data set. Hence it is an important task to decide for any given set of data which method produces the best results. Selecting the best approach can be one of the most challenging parts of performing statistical learning in practice.

In this section, we discuss some of the most important concepts that arise in selecting a statistical learning procedure for a specific data set. As the book progresses, we will explain how the concepts presented here can be applied in practice.

2.2.1 Measuring the Quality of Fit

In order to evaluate the performance of a statistical learning method on a given data set, we need some way to measure how well its predictions actually match the observed data. That is, we need to quantify the extent to which the predicted response value for a given observation is close to the true response value for that observation. In the regression setting, the most commonly-used measure is the *mean squared error* (MSE), given by

mean squared error

$$\text{MSE} = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{f}(x_i))^2, \tag{2.5}$$

where $\hat{f}(x_i)$ is the prediction that $\hat{f}$ gives for the ith observation. The MSE will be small if the predicted responses are very close to the true responses,

and will be large if for some of the observations, the predicted and true responses differ substantially.

The MSE in (2.5) is computed using the training data that was used to fit the model, and so should more accurately be referred to as the *training MSE*. But in general, we do not really care how well the method works on the training data. Rather, *we are interested in the accuracy of the predictions that we obtain when we apply our method to previously unseen test data*. Why is this what we care about? Suppose that we are interested in developing an algorithm to predict a stock's price based on previous stock returns. We can train the method using stock returns from the past 6 months. But we don't really care how well our method predicts last week's stock price. We instead care about how well it will predict tomorrow's price or next month's price. On a similar note, suppose that we have clinical measurements (e.g. weight, blood pressure, height, age, family history of disease) for a number of patients, as well as information about whether each patient has diabetes. We can use these patients to train a statistical learning method to predict risk of diabetes based on clinical measurements. In practice, we want this method to accurately predict diabetes risk for *future patients* based on their clinical measurements. We are not very interested in whether or not the method accurately predicts diabetes risk for patients used to train the model, since we already know which of those patients have diabetes.

training MSE

test data

To state it more mathematically, suppose that we fit our statistical learning method on our training observations $\{(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)\}$, and we obtain the estimate $\hat{f}$. We can then compute $\hat{f}(x_1), \hat{f}(x_2), \ldots, \hat{f}(x_n)$. If these are approximately equal to $y_1, y_2, \ldots, y_n$, then the training MSE given by (2.5) is small. However, we are really not interested in whether $\hat{f}(x_i) \approx y_i$; instead, we want to know whether $\hat{f}(x_0)$ is approximately equal to y_0, where (x_0, y_0) is a *previously unseen test observation not used to train the statistical learning method*. We want to choose the method that gives the lowest *test MSE*, as opposed to the lowest training MSE. In other words, if we had a large number of test observations, we could compute

test MSE

$$\text{Ave}(y_0 - \hat{f}(x_0))^2, \tag{2.6}$$

the average squared prediction error for these test observations (x_0, y_0). We'd like to select the model for which this quantity is as small as possible.

How can we go about trying to select a method that minimizes the test MSE? In some settings, we may have a test data set available—that is, we may have access to a set of observations that were not used to train the statistical learning method. We can then simply evaluate (2.6) on the test observations, and select the learning method for which the test MSE is smallest. But what if no test observations are available? In that case, one might imagine simply selecting a statistical learning method that minimizes the training MSE (2.5). This seems like it might be a sensible approach,

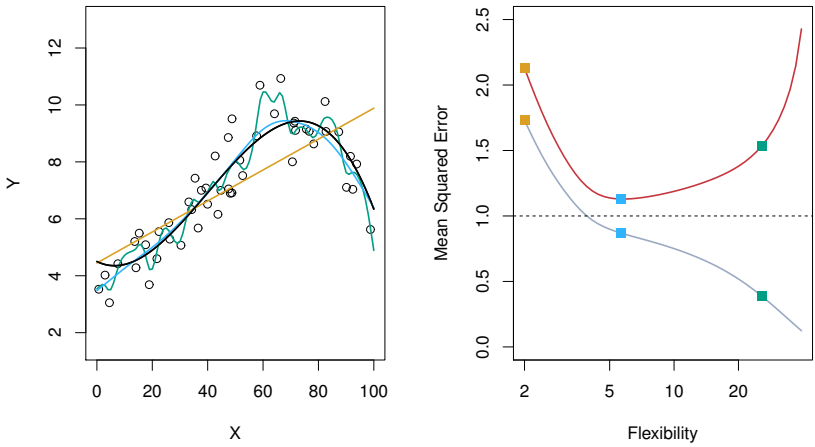


FIGURE 2.9. Left: *Data simulated from f, shown in black. Three estimates of f are shown: the linear regression line (orange curve), and two smoothing spline fits (blue and green curves).* Right: *Training MSE (grey curve), test MSE (red curve), and minimum possible test MSE over all methods (dashed line). Squares represent the training and test MSEs for the three fits shown in the left-hand panel.*

since the training MSE and the test MSE appear to be closely related. Unfortunately, there is a fundamental problem with this strategy: there is no guarantee that the method with the lowest training MSE will also have the lowest test MSE. Roughly speaking, the problem is that many statistical methods specifically estimate coefficients so as to minimize the training set MSE. For these methods, the training set MSE can be quite small, but the test MSE is often much larger.

Figure 2.9 illustrates this phenomenon on a simple example. In the left-hand panel of Figure 2.9, we have generated observations from (2.1) with the true f given by the black curve. The orange, blue and green curves illustrate three possible estimates for f obtained using methods with increasing levels of flexibility. The orange line is the linear regression fit, which is relatively inflexible. The blue and green curves were produced using *smoothing splines*, discussed in Chapter 7, with different levels of smoothness. It is clear that as the level of flexibility increases, the curves fit the observed data more closely. The green curve is the most flexible and matches the data very well; however, we observe that it fits the true f (shown in black) poorly because it is too wiggly. By adjusting the level of flexibility of the smoothing spline fit, we can produce many different fits to this data.

smoothing spline

We now move on to the right-hand panel of Figure 2.9. The grey curve displays the average training MSE as a function of flexibility, or more formally the *degrees of freedom*, for a number of smoothing splines. The degrees of freedom is a quantity that summarizes the flexibility of a curve;

degrees of freedom

it is discussed more fully in Chapter 7. The orange, blue and green squares indicate the MSEs associated with the corresponding curves in the left-hand panel. A more restricted and hence smoother curve has fewer degrees of freedom than a wiggly curve—note that in Figure 2.9, linear regression is at the most restrictive end, with two degrees of freedom. The training MSE declines monotonically as flexibility increases. In this example the true f is non-linear, and so the orange linear fit is not flexible enough to estimate f well. The green curve has the lowest training MSE of all three methods, since it corresponds to the most flexible of the three curves fit in the left-hand panel.

In this example, we know the true function f, and so we can also compute the test MSE over a very large test set, as a function of flexibility. (Of course, in general f is unknown, so this will not be possible.) The test MSE is displayed using the red curve in the right-hand panel of Figure 2.9. As with the training MSE, the test MSE initially declines as the level of flexibility increases. However, at some point the test MSE levels off and then starts to increase again. Consequently, the orange and green curves both have high test MSE. The blue curve minimizes the test MSE, which should not be surprising given that visually it appears to estimate f the best in the left-hand panel of Figure 2.9. The horizontal dashed line indicates $\text{Var}(\epsilon)$, the irreducible error in (2.3), which corresponds to the lowest achievable test MSE among all possible methods. Hence, the smoothing spline represented by the blue curve is close to optimal.

In the right-hand panel of Figure 2.9, as the flexibility of the statistical learning method increases, we observe a monotone decrease in the training MSE and a *U-shape* in the test MSE. This is a fundamental property of statistical learning that holds regardless of the particular data set at hand and regardless of the statistical method being used. As model flexibility increases, the training MSE will decrease, but the test MSE may not. When a given method yields a small training MSE but a large test MSE, we are said to be *overfitting* the data. This happens because our statistical learning procedure is working too hard to find patterns in the training data, and may be picking up some patterns that are just caused by random chance rather than by true properties of the unknown function f. When we overfit the training data, the test MSE will be very large because the supposed patterns that the method found in the training data simply don't exist in the test data. Note that regardless of whether or not overfitting has occurred, we almost always expect the training MSE to be smaller than the test MSE because most statistical learning methods either directly or indirectly seek to minimize the training MSE. Overfitting refers specifically to the case in which a less flexible model would have yielded a smaller test MSE.

Figure 2.10 provides another example in which the true f is approximately linear. Again we observe that the training MSE decreases monotonically as the model flexibility increases, and that there is a U-shape in

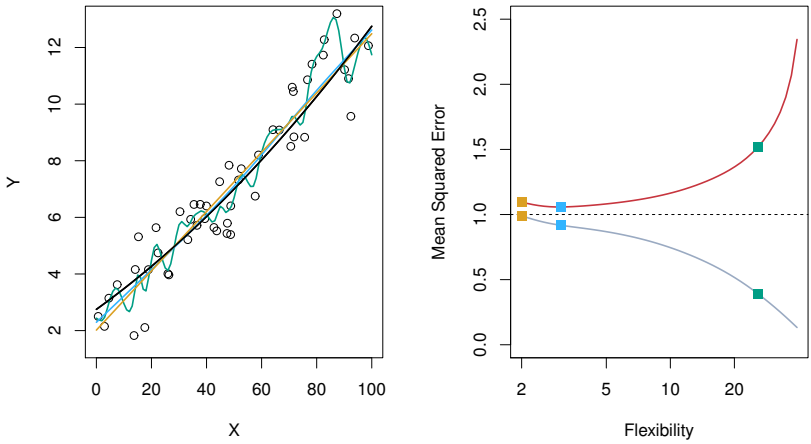


FIGURE 2.10. *Details are as in Figure 2.9, using a different true f that is much closer to linear. In this setting, linear regression provides a very good fit to the data.*

the test MSE. However, because the truth is close to linear, the test MSE only decreases slightly before increasing again, so that the orange least squares fit is substantially better than the highly flexible green curve. Finally, Figure 2.11 displays an example in which f is highly non-linear. The training and test MSE curves still exhibit the same general patterns, but now there is a rapid decrease in both curves before the test MSE starts to increase slowly.

In practice, one can usually compute the training MSE with relative ease, but estimating the test MSE is considerably more difficult because usually no test data are available. As the previous three examples illustrate, the flexibility level corresponding to the model with the minimal test MSE can vary considerably among data sets. Throughout this book, we discuss a variety of approaches that can be used in practice to estimate this minimum point. One important method is *cross-validation* (Chapter 5), which is a method for estimating the test MSE using the training data.

cross-validation

2.2.2 The Bias-Variance Trade-Off

The U-shape observed in the test MSE curves (Figures 2.9–2.11) turns out to be the result of two competing properties of statistical learning methods. Though the mathematical proof is beyond the scope of this book, it is possible to show that the expected test MSE, for a given value x_0, can always be decomposed into the sum of three fundamental quantities: the *variance* of $\hat{f}(x_0)$, the squared *bias* of $\hat{f}(x_0)$ and the variance of the error

variance
bias

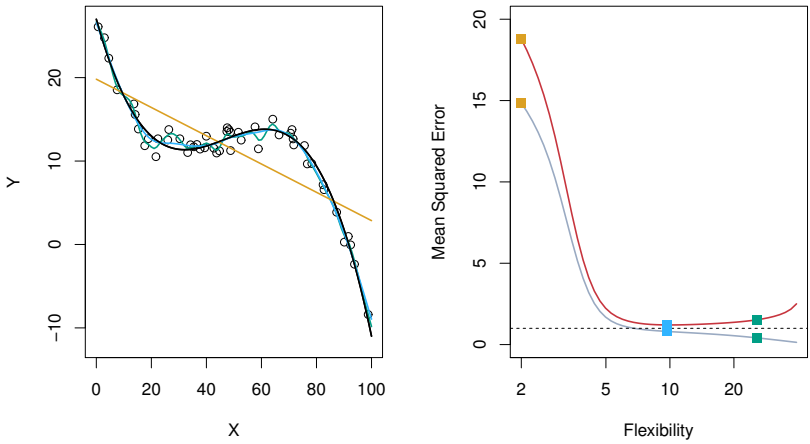


FIGURE 2.11. *Details are as in Figure 2.9, using a different f that is far from linear. In this setting, linear regression provides a very poor fit to the data.*

terms ϵ. That is,

$$E\left(y_0 - \hat{f}(x_0)\right)^2 = \text{Var}(\hat{f}(x_0)) + [\text{Bias}(\hat{f}(x_0))]^2 + \text{Var}(\epsilon). \tag{2.7}$$

Here the notation $E\left(y_0 - \hat{f}(x_0)\right)^2$ defines the *expected test MSE* at x_0, and refers to the average test MSE that we would obtain if we repeatedly estimated f using a large number of training sets, and tested each at x_0. The overall expected test MSE can be computed by averaging $E\left(y_0 - \hat{f}(x_0)\right)^2$ over all possible values of x_0 in the test set.

expected test MSE

Equation 2.7 tells us that in order to minimize the expected test error, we need to select a statistical learning method that simultaneously achieves *low variance* and *low bias*. Note that variance is inherently a nonnegative quantity, and squared bias is also nonnegative. Hence, we see that the expected test MSE can never lie below $\text{Var}(\epsilon)$, the irreducible error from (2.3).

What do we mean by the *variance* and *bias* of a statistical learning method? *Variance* refers to the amount by which $\hat{f}$ would change if we estimated it using a different training data set. Since the training data are used to fit the statistical learning method, different training data sets will result in a different $\hat{f}$. But ideally the estimate for f should not vary too much between training sets. However, if a method has high variance then small changes in the training data can result in large changes in $\hat{f}$. In general, more flexible statistical methods have higher variance. Consider the green and orange curves in Figure 2.9. The flexible green curve is following the observations very closely. It has high variance because changing any

one of these data points may cause the estimate $\hat{f}$ to change considerably. In contrast, the orange least squares line is relatively inflexible and has low variance, because moving any single observation will likely cause only a small shift in the position of the line.

On the other hand, *bias* refers to the error that is introduced by approximating a real-life problem, which may be extremely complicated, by a much simpler model. For example, linear regression assumes that there is a linear relationship between Y and $X_1, X_2, \ldots, X_p$. It is unlikely that any real-life problem truly has such a simple linear relationship, and so performing linear regression will undoubtedly result in some bias in the estimate of f. In Figure 2.11, the true f is substantially non-linear, so no matter how many training observations we are given, it will not be possible to produce an accurate estimate using linear regression. In other words, linear regression results in high bias in this example. However, in Figure 2.10 the true f is very close to linear, and so given enough data, it should be possible for linear regression to produce an accurate estimate. Generally, more flexible methods result in less bias.

As a general rule, as we use more flexible methods, the variance will increase and the bias will decrease. The relative rate of change of these two quantities determines whether the test MSE increases or decreases. As we increase the flexibility of a class of methods, the bias tends to initially decrease faster than the variance increases. Consequently, the expected test MSE declines. However, at some point increasing flexibility has little impact on the bias but starts to significantly increase the variance. When this happens the test MSE increases. Note that we observed this pattern of decreasing test MSE followed by increasing test MSE in the right-hand panels of Figures 2.9–2.11.

The three plots in Figure 2.12 illustrate Equation 2.7 for the examples in Figures 2.9–2.11. In each case the blue solid curve represents the squared bias, for different levels of flexibility, while the orange curve corresponds to the variance. The horizontal dashed line represents $\mathrm{Var}(\epsilon)$, the irreducible error. Finally, the red curve, corresponding to the test set MSE, is the sum of these three quantities. In all three cases, the variance increases and the bias decreases as the method's flexibility increases. However, the flexibility level corresponding to the optimal test MSE differs considerably among the three data sets, because the squared bias and variance change at different rates in each of the data sets. In the left-hand panel of Figure 2.12, the bias initially decreases rapidly, resulting in an initial sharp decrease in the expected test MSE. On the other hand, in the center panel of Figure 2.12 the true f is close to linear, so there is only a small decrease in bias as flexibility increases, and the test MSE only declines slightly before increasing rapidly as the variance increases. Finally, in the right-hand panel of Figure 2.12, as flexibility increases, there is a dramatic decline in bias because the true f is very non-linear. There is also very little increase in variance

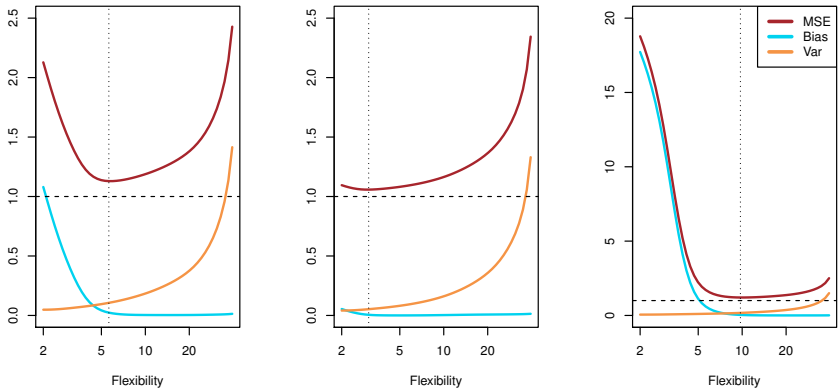


FIGURE 2.12. *Squared bias (blue curve), variance (orange curve), Var(ϵ) (dashed line), and test MSE (red curve) for the three data sets in Figures 2.9–2.11. The vertical dotted line indicates the flexibility level corresponding to the smallest test MSE.*

as flexibility increases. Consequently, the test MSE declines substantially before experiencing a small increase as model flexibility increases.

The relationship between bias, variance, and test set MSE given in Equation 2.7 and displayed in Figure 2.12 is referred to as the *bias-variance trade-off*. Good test set performance of a statistical learning method requires low variance as well as low squared bias. This is referred to as a trade-off because it is easy to obtain a method with extremely low bias but high variance (for instance, by drawing a curve that passes through every single training observation) or a method with very low variance but high bias (by fitting a horizontal line to the data). The challenge lies in finding a method for which both the variance and the squared bias are low. This trade-off is one of the most important recurring themes in this book.

bias-variance trade-off

In a real-life situation in which f is unobserved, it is generally not possible to explicitly compute the test MSE, bias, or variance for a statistical learning method. Nevertheless, one should always keep the bias-variance trade-off in mind. In this book we explore methods that are extremely flexible and hence can essentially eliminate bias. However, this does not guarantee that they will outperform a much simpler method such as linear regression. To take an extreme example, suppose that the true f is linear. In this situation linear regression will have no bias, making it very hard for a more flexible method to compete. In contrast, if the true f is highly non-linear and we have an ample number of training observations, then we may do better using a highly flexible approach, as in Figure 2.11. In Chapter 5 we discuss cross-validation, which is a way to estimate the test MSE using the training data.

2.2.3 The Classification Setting

Thus far, our discussion of model accuracy has been focused on the regression setting. But many of the concepts that we have encountered, such as the bias-variance trade-off, transfer over to the classification setting with only some modifications due to the fact that y_i is no longer quantitative. Suppose that we seek to estimate f on the basis of training observations $\{(x_1, y_1), \ldots, (x_n, y_n)\}$, where now $y_1, \ldots, y_n$ are qualitative. The most common approach for quantifying the accuracy of our estimate $\hat{f}$ is the training *error rate*, the proportion of mistakes that are made if we apply our estimate $\hat{f}$ to the training observations:

error rate

$$\frac{1}{n}\sum_{i=1}^{n} I(y_i \neq \hat{y}_i). \tag{2.8}$$

Here $\hat{y}_i$ is the predicted class label for the ith observation using $\hat{f}$. And $I(y_i \neq \hat{y}_i)$ is an *indicator variable* that equals 1 if $y_i \neq \hat{y}_i$ and zero if $y_i = \hat{y}_i$. If $I(y_i \neq \hat{y}_i) = 0$ then the ith observation was classified correctly by our classification method; otherwise it was misclassified. Hence Equation 2.8 computes the fraction of incorrect classifications.

indicator variable

Equation 2.8 is referred to as the *training error* rate because it is computed based on the data that was used to train our classifier. As in the regression setting, we are most interested in the error rates that result from applying our classifier to test observations that were not used in training. The *test error* rate associated with a set of test observations of the form (x_0, y_0) is given by

training error

test error

$$\text{Ave}\left(I(y_0 \neq \hat{y}_0)\right), \tag{2.9}$$

where $\hat{y}_0$ is the predicted class label that results from applying the classifier to the test observation with predictor x_0. A *good* classifier is one for which the test error (2.9) is smallest.

The Bayes Classifier

It is possible to show (though the proof is outside of the scope of this book) that the test error rate given in (2.9) is minimized, on average, by a very simple classifier that *assigns each observation to the most likely class, given its predictor values*. In other words, we should simply assign a test observation with predictor vector x_0 to the class j for which

$$\Pr(Y = j | X = x_0) \tag{2.10}$$

is largest. Note that (2.10) is a *conditional probability*: it is the probability that $Y = j$, given the observed predictor vector x_0. This very simple classifier is called the *Bayes classifier*. In a two-class problem where there are only two possible response values, say *class 1* or *class 2*, the Bayes classifier

conditional probability

Bayes classifier

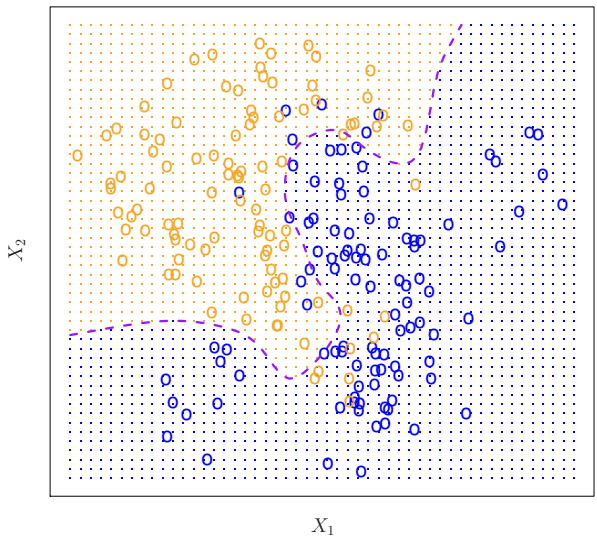


FIGURE 2.13. *A simulated data set consisting of* 100 *observations in each of two groups, indicated in blue and in orange. The purple dashed line represents the Bayes decision boundary. The orange background grid indicates the region in which a test observation will be assigned to the orange class, and the blue background grid indicates the region in which a test observation will be assigned to the blue class.*

corresponds to predicting class one if $\Pr(Y = 1|X = x_0) > 0.5$, and class two otherwise.

Figure 2.13 provides an example using a simulated data set in a two-dimensional space consisting of predictors X_1 and X_2. The orange and blue circles correspond to training observations that belong to two different classes. For each value of X_1 and X_2, there is a different probability of the response being orange or blue. Since this is simulated data, we know how the data were generated and we can calculate the conditional probabilities for each value of X_1 and X_2. The orange shaded region reflects the set of points for which $\Pr(Y = \text{orange}|X)$ is greater than 50 %, while the blue shaded region indicates the set of points for which the probability is below 50 %. The purple dashed line represents the points where the probability is exactly 50 %. This is called the *Bayes decision boundary*. The Bayes classifier's prediction is determined by the Bayes decision boundary; an observation that falls on the orange side of the boundary will be assigned to the orange class, and similarly an observation on the blue side of the boundary will be assigned to the blue class.

Bayes decision boundary

The Bayes classifier produces the lowest possible test error rate, called the *Bayes error rate*. Since the Bayes classifier will always choose the class for which (2.10) is largest, the error rate will be $1 - \max_j \Pr(Y = j|X = x_0)$

Bayes error rate

at $X = x_0$. In general, the overall Bayes error rate is given by

$$1 - E\left(\max_j \Pr(Y = j|X)\right), \tag{2.11}$$

where the expectation averages the probability over all possible values of X. For our simulated data, the Bayes error rate is 0.133. It is greater than zero, because the classes overlap in the true population, which implies that $\max_j \Pr(Y = j|X = x_0) < 1$ for some values of x_0. The Bayes error rate is analogous to the irreducible error, discussed earlier.

K-Nearest Neighbors

In theory we would always like to predict qualitative responses using the Bayes classifier. But for real data, we do not know the conditional distribution of Y given X, and so computing the Bayes classifier is impossible. Therefore, the Bayes classifier serves as an unattainable gold standard against which to compare other methods. Many approaches attempt to estimate the conditional distribution of Y given X, and then classify a given observation to the class with highest *estimated* probability. One such method is the *K-nearest neighbors* (KNN) classifier. Given a positive integer K and a test observation x_0, the KNN classifier first identifies the K points in the training data that are closest to x_0, represented by $\mathcal{N}_0$. It then estimates the conditional probability for class j as the fraction of points in $\mathcal{N}_0$ whose response values equal j:

K-nearest neighbors

$$\Pr(Y = j|X = x_0) = \frac{1}{K} \sum_{i \in \mathcal{N}_0} I(y_i = j). \tag{2.12}$$

Finally, KNN classifies the test observation x_0 to the class with the largest probability from (2.12).

Figure 2.14 provides an illustrative example of the KNN approach. In the left-hand panel, we have plotted a small training data set consisting of six blue and six orange observations. Our goal is to make a prediction for the point labeled by the black cross. Suppose that we choose $K = 3$. Then KNN will first identify the three observations that are closest to the cross. This neighborhood is shown as a circle. It consists of two blue points and one orange point, resulting in estimated probabilities of 2/3 for the blue class and 1/3 for the orange class. Hence KNN will predict that the black cross belongs to the blue class. In the right-hand panel of Figure 2.14 we have applied the KNN approach with $K = 3$ at all of the possible values for X_1 and X_2, and have drawn in the corresponding KNN decision boundary.

Despite the fact that it is a very simple approach, KNN can often produce classifiers that are surprisingly close to the optimal Bayes classifier. Figure 2.15 displays the KNN decision boundary, using $K = 10$, when applied to the larger simulated data set from Figure 2.13. Notice that even

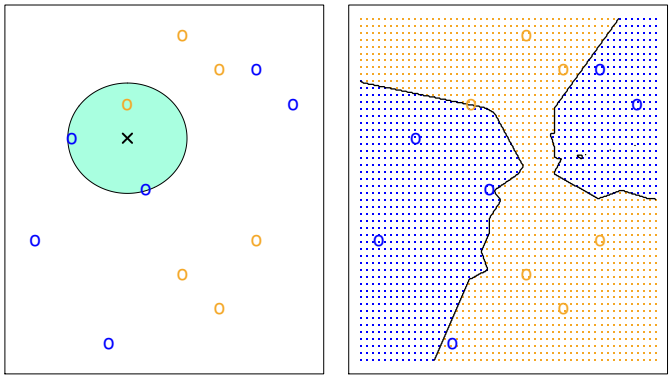


FIGURE 2.14. *The KNN approach, using $K = 3$, is illustrated in a simple situation with six blue observations and six orange observations.* Left: *a test observation at which a predicted class label is desired is shown as a black cross. The three closest points to the test observation are identified, and it is predicted that the test observation belongs to the most commonly-occurring class, in this case blue.* Right: *The KNN decision boundary for this example is shown in black. The blue grid indicates the region in which a test observation will be assigned to the blue class, and the orange grid indicates the region in which it will be assigned to the orange class.*

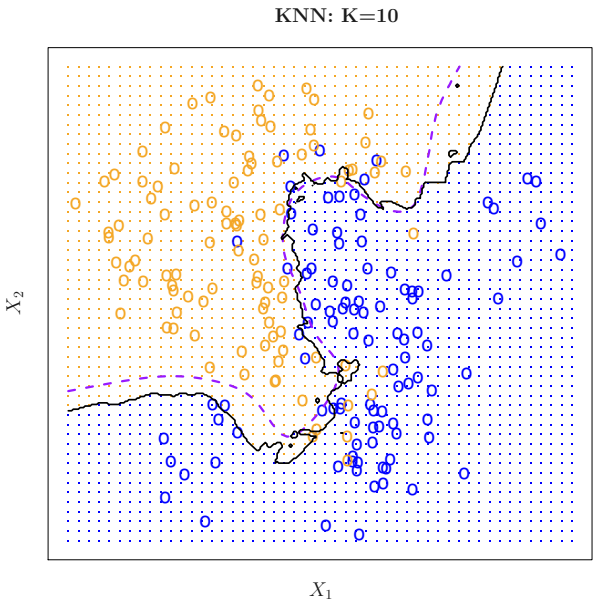


FIGURE 2.15. *The black curve indicates the KNN decision boundary on the data from Figure 2.13, using $K = 10$. The Bayes decision boundary is shown as a purple dashed line. The KNN and Bayes decision boundaries are very similar.*

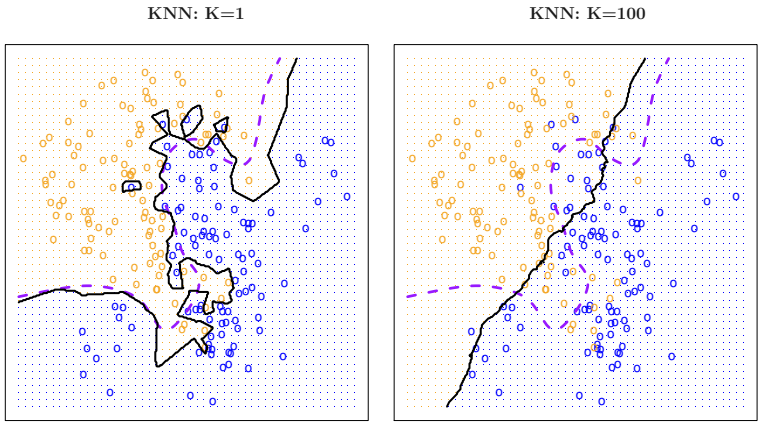


FIGURE 2.16. *A comparison of the KNN decision boundaries (solid black curves) obtained using $K = 1$ and $K = 100$ on the data from Figure 2.13. With $K = 1$, the decision boundary is overly flexible, while with $K = 100$ it is not sufficiently flexible. The Bayes decision boundary is shown as a purple dashed line.*

though the true distribution is not known by the KNN classifier, the KNN decision boundary is very close to that of the Bayes classifier. The test error rate using KNN is 0.1363, which is close to the Bayes error rate of 0.1304.

The choice of K has a drastic effect on the KNN classifier obtained. Figure 2.16 displays two KNN fits to the simulated data from Figure 2.13, using $K = 1$ and $K = 100$. When $K = 1$, the decision boundary is overly flexible and finds patterns in the data that don't correspond to the Bayes decision boundary. This corresponds to a classifier that has low bias but very high variance. As K grows, the method becomes less flexible and produces a decision boundary that is close to linear. This corresponds to a low-variance but high-bias classifier. On this simulated data set, neither $K = 1$ nor $K = 100$ give good predictions: they have test error rates of 0.1695 and 0.1925, respectively.

Just as in the regression setting, there is not a strong relationship between the training error rate and the test error rate. With $K = 1$, the KNN training error rate is 0, but the test error rate may be quite high. In general, as we use more flexible classification methods, the training error rate will decline but the test error rate may not. In Figure 2.17, we have plotted the KNN test and training errors as a function of $1/K$. As $1/K$ increases, the method becomes more flexible. As in the regression setting, the training error rate consistently declines as the flexibility increases. However, the test error exhibits a characteristic U-shape, declining at first (with a minimum at approximately $K = 10$) before increasing again when the method becomes excessively flexible and overfits.

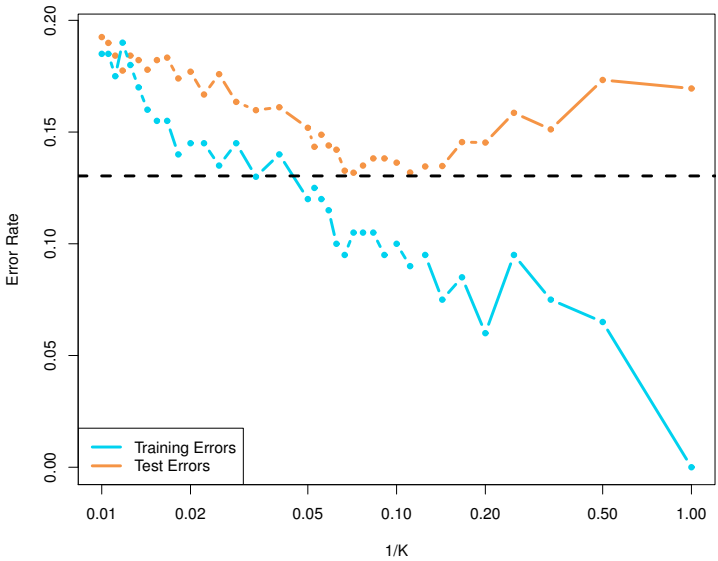


FIGURE 2.17. *The KNN training error rate (blue, 200 observations) and test error rate (orange, 5,000 observations) on the data from Figure 2.13, as the level of flexibility (assessed using* $1/K$ *on the log scale) increases, or equivalently as the number of neighbors* K *decreases. The black dashed line indicates the Bayes error rate. The jumpiness of the curves is due to the small size of the training data set.*

In both the regression and classification settings, choosing the correct level of flexibility is critical to the success of any statistical learning method. The bias-variance tradeoff, and the resulting U-shape in the test error, can make this a difficult task. In Chapter 5, we return to this topic and discuss various methods for estimating test error rates and thereby choosing the optimal level of flexibility for a given statistical learning method.

2.3 Lab: Introduction to R

In this lab, we will introduce some simple `R` commands. The best way to learn a new language is to try out the commands. `R` can be downloaded from

`http://cran.r-project.org/`

We recommend that you run `R` within an integrated development environment (IDE) such as `RStudio`, which can be freely downloaded from

`http://rstudio.com`

The RStudio website also provides a cloud-based version of R, which does not require installing any software.

2.3.1 Basic Commands

R uses *functions* to perform operations. To run a function called funcname, we type funcname(input1, input2), where the inputs (or *arguments*) input1 and input2 tell R how to run the function. A function can have any number of inputs. For example, to create a vector of numbers, we use the function c() (for *concatenate*). Any numbers inside the parentheses are joined together. The following command instructs R to join together the numbers 1, 3, 2, and 5, and to save them as a *vector* named x. When we type x, it gives us back the vector.

function
argument
c()
vector

```
> x <- c(1, 3, 2, 5)
> x
[1] 1 3 2 5
```

Note that the > is not part of the command; rather, it is printed by R to indicate that it is ready for another command to be entered. We can also save things using = rather than <-:

```
> x = c(1, 6, 2)
> x
[1] 1 6 2
> y = c(1, 4, 3)
```

Hitting the *up* arrow multiple times will display the previous commands, which can then be edited. This is useful since one often wishes to repeat a similar command. In addition, typing ?funcname will always cause R to open a new help file window with additional information about the function funcname().

We can tell R to add two sets of numbers together. It will then add the first number from x to the first number from y, and so on. However, x and y should be the same length. We can check their length using the length() function.

length()

```
> length(x)
[1] 3
> length(y)
[1] 3
> x + y
[1]  2 10  5
```

The ls() function allows us to look at a list of all of the objects, such as data and functions, that we have saved so far. The rm() function can be used to delete any that we don't want.

ls()
rm()

```
> ls()
[1] "x" "y"
> rm(x, y)
```

```
> ls()
character(0)
```

It's also possible to remove all objects at once:

```
> rm(list = ls())
```

The `matrix()` function can be used to create a matrix of numbers. Before we use the `matrix()` function, we can learn more about it: `matrix()`

```
> ?matrix
```

The help file reveals that the `matrix()` function takes a number of inputs, but for now we focus on the first three: the data (the entries in the matrix), the number of rows, and the number of columns. First, we create a simple matrix.

```
> x <- matrix(data = c(1, 2, 3, 4), nrow = 2, ncol = 2)
> x
     [,1] [,2]
[1,]    1    3
[2,]    2    4
```

Note that we could just as well omit typing `data=`, `nrow=`, and `ncol=` in the `matrix()` command above: that is, we could just type

```
> x <- matrix(c(1, 2, 3, 4), 2, 2)
```

and this would have the same effect. However, it can sometimes be useful to specify the names of the arguments passed in, since otherwise `R` will assume that the function arguments are passed into the function in the same order that is given in the function's help file. As this example illustrates, by default `R` creates matrices by successively filling in columns. Alternatively, the `byrow = TRUE` option can be used to populate the matrix in order of the rows.

```
> matrix(c(1, 2, 3, 4), 2, 2, byrow = TRUE)
     [,1] [,2]
[1,]    1    2
[2,]    3    4
```

Notice that in the above command we did not assign the matrix to a value such as `x`. In this case the matrix is printed to the screen but is not saved for future calculations. The `sqrt()` function returns the square root of each element of a vector or matrix. The command `x^2` raises each element of `x` to the power `2`; any powers are possible, including fractional or negative powers. `sqrt()`

```
> sqrt(x)
     [,1] [,2]
[1,] 1.00 1.73
[2,] 1.41 2.00
> x^2
     [,1] [,2]
[1,]    1    9
[2,]    4   16
```

The `rnorm()` function generates a vector of random normal variables, with first argument `n` the sample size. Each time we call this function, we will get a different answer. Here we create two correlated sets of numbers, `x` and `y`, and use the `cor()` function to compute the correlation between them.

`rnorm()`

`cor()`

```
> x <- rnorm(50)
> y <- x + rnorm(50, mean = 50, sd = .1)
> cor(x, y)
[1] 0.995
```

By default, `rnorm()` creates standard normal random variables with a mean of 0 and a standard deviation of 1. However, the mean and standard deviation can be altered using the `mean` and `sd` arguments, as illustrated above. Sometimes we want our code to reproduce the exact same set of random numbers; we can use the `set.seed()` function to do this. The `set.seed()` function takes an (arbitrary) integer argument.

`set.seed()`

```
> set.seed(1303)
> rnorm(50)
[1] -1.1440  1.3421  2.1854  0.5364  0.0632  0.5022 -0.0004
. . .
```

We use `set.seed()` throughout the labs whenever we perform calculations involving random quantities. In general this should allow the user to reproduce our results. However, as new versions of `R` become available, small discrepancies may arise between this book and the output from `R`.

The `mean()` and `var()` functions can be used to compute the mean and variance of a vector of numbers. Applying `sqrt()` to the output of `var()` will give the standard deviation. Or we can simply use the `sd()` function.

`mean()`

`var()`

`sd()`

```
> set.seed(3)
> y <- rnorm(100)
> mean(y)
[1] 0.0110
> var(y)
[1] 0.7329
> sqrt(var(y))
[1] 0.8561
> sd(y)
[1] 0.8561
```

2.3.2 Graphics

The `plot()` function is the primary way to plot data in `R`. For instance, `plot(x, y)` produces a scatterplot of the numbers in `x` versus the numbers in `y`. There are many additional options that can be passed in to the `plot()` function. For example, passing in the argument `xlab` will result in a label on the x-axis. To find out more information about the `plot()` function, type `?plot`.

`plot()`

```
> x <- rnorm(100)
> y <- rnorm(100)
> plot(x, y)
> plot(x, y, xlab = "this is the x-axis",
    ylab = "this is the y-axis",
    main = "Plot of X vs Y")
```

We will often want to save the output of an R plot. The command that we use to do this will depend on the file type that we would like to create. For instance, to create a pdf, we use the `pdf()` function, and to create a jpeg, we use the `jpeg()` function.

`pdf()`
`jpeg()`

```
> pdf("Figure.pdf")
> plot(x, y, col = "green")
> dev.off()
null device
          1
```

The function `dev.off()` indicates to R that we are done creating the plot. Alternatively, we can simply copy the plot window and paste it into an appropriate file type, such as a Word document.

`dev.off()`

The function `seq()` can be used to create a sequence of numbers. For instance, `seq(a, b)` makes a vector of integers between `a` and `b`. There are many other options: for instance, `seq(0, 1, length = 10)` makes a sequence of `10` numbers that are equally spaced between `0` and `1`. Typing `3:11` is a shorthand for `seq(3, 11)` for integer arguments.

`seq()`

```
> x <- seq(1, 10)
> x
 [1]  1  2  3  4  5  6  7  8  9 10
> x <- 1:10
> x
 [1]  1  2  3  4  5  6  7  8  9 10
> x <- seq(-pi, pi, length = 50)
```

We will now create some more sophisticated plots. The `contour()` function produces a *contour plot* in order to represent three-dimensional data; it is like a topographical map. It takes three arguments:

`contour()`
contour plot

1. A vector of the `x` values (the first dimension),
2. A vector of the `y` values (the second dimension), and
3. A matrix whose elements correspond to the `z` value (the third dimension) for each pair of (`x`, `y`) coordinates.

As with the `plot()` function, there are many other inputs that can be used to fine-tune the output of the `contour()` function. To learn more about these, take a look at the help file by typing `?contour`.

```
> y <- x
> f <- outer(x, y, function(x, y) cos(y) / (1 + x^2))
> contour(x, y, f)
> contour(x, y, f, nlevels = 45, add = T)
```

```
> fa <- (f - t(f)) / 2
> contour(x, y, fa, nlevels = 15)
```

The `image()` function works the same way as `contour()`, except that it produces a color-coded plot whose colors depend on the `z` value. This is known as a *heatmap*, and is sometimes used to plot temperature in weather forecasts. Alternatively, `persp()` can be used to produce a three-dimensional plot. The arguments `theta` and `phi` control the angles at which the plot is viewed.

image()

heatmap

persp()

```
> image(x, y, fa)
> persp(x, y, fa)
> persp(x, y, fa, theta = 30)
> persp(x, y, fa, theta = 30, phi = 20)
> persp(x, y, fa, theta = 30, phi = 70)
> persp(x, y, fa, theta = 30, phi = 40)
```

2.3.3 Indexing Data

We often wish to examine part of a set of data. Suppose that our data is stored in the matrix `A`.

```
> A <- matrix(1:16, 4, 4)
> A
     [,1] [,2] [,3] [,4]
[1,]    1    5    9   13
[2,]    2    6   10   14
[3,]    3    7   11   15
[4,]    4    8   12   16
```

Then, typing

```
> A[2, 3]
[1] 10
```

will select the element corresponding to the second row and the third column. The first number after the open-bracket symbol `[` always refers to the row, and the second number always refers to the column. We can also select multiple rows and columns at a time, by providing vectors as the indices.

```
> A[c(1, 3), c(2, 4)]
     [,1] [,2]
[1,]    5   13
[2,]    7   15
> A[1:3, 2:4]
     [,1] [,2] [,3]
[1,]    5    9   13
[2,]    6   10   14
[3,]    7   11   15
> A[1:2, ]
     [,1] [,2] [,3] [,4]
[1,]    1    5    9   13
[2,]    2    6   10   14
```

```
> A[, 1:2]
     [,1] [,2]
[1,]    1    5
[2,]    2    6
[3,]    3    7
[4,]    4    8
```

The last two examples include either no index for the columns or no index for the rows. These indicate that R should include all columns or all rows, respectively. R treats a single row or column of a matrix as a vector.

```
> A[1, ]
[1]  1  5  9 13
```

The use of a negative sign - in the index tells R to keep all rows or columns except those indicated in the index.

```
> A[-c(1, 3), ]
     [,1] [,2] [,3] [,4]
[1,]    2    6   10   14
[2,]    4    8   12   16
> A[-c(1, 3), -c(1, 3, 4)]
[1] 6 8
```

The dim() function outputs the number of rows followed by the number of columns of a given matrix.

dim()

```
> dim(A)
[1] 4 4
```

2.3.4 Loading Data

For most analyses, the first step involves importing a data set into R. The read.table() function is one of the primary ways to do this. The help file contains details about how to use this function. We can use the function write.table() to export data.

read.table()

write.table()

Before attempting to load a data set, we must make sure that R knows to search for the data in the proper directory. For example, on a Windows system one could select the directory using the Change dir... option under the File menu. However, the details of how to do this depend on the operating system (e.g. Windows, Mac, Unix) that is being used, and so we do not give further details here.

We begin by loading in the Auto data set. This data is part of the ISLR2 library, discussed in Chapter 3. To illustrate the read.table() function, we load it now from a text file, Auto.data, which you can find on the textbook website. The following command will load the Auto.data file into R and store it as an object called Auto, in a format referred to as a *data frame*. Once the data has been loaded, the View() function can be used to view

data frame

it in a spreadsheet-like window.[1] The `head()` function can also be used to view the first few rows of the data.

```
> Auto <- read.table("Auto.data")
> View(Auto)
> head(Auto)
    V1         V2           V3          V4     V5
1  mpg cylinders displacement horsepower weight
2 18.0         8        307.0      130.0  3504.
3 15.0         8        350.0      165.0  3693.
4 18.0         8        318.0      150.0  3436.
5 16.0         8        304.0      150.0  3433.
6 17.0         8        302.0      140.0  3449.
            V6   V7     V8                          V9
1 acceleration year origin                        name
2         12.0   70      1 chevrolet chevelle malibu
3         11.5   70      1          buick skylark 320
4         11.0   70      1         plymouth satellite
5         12.0   70      1              amc rebel sst
6         10.5   70      1                ford torino
```

Note that Auto.data is simply a text file, which you could alternatively open on your computer using a standard text editor. It is often a good idea to view a data set using a text editor or other software such as Excel before loading it into `R`.

This particular data set has not been loaded correctly, because `R` has assumed that the variable names are part of the data and so has included them in the first row. The data set also includes a number of missing observations, indicated by a question mark `?`. Missing values are a common occurrence in real data sets. Using the option `header = T` (or `header = TRUE`) in the `read.table()` function tells `R` that the first line of the file contains the variable names, and using the option `na.strings` tells `R` that any time it sees a particular character or set of characters (such as a question mark), it should be treated as a missing element of the data matrix.

```
> Auto <- read.table("Auto.data", header = T, na.strings = "?",
    stringsAsFactors = T)
> View(Auto)
```

The `stringsAsFactors = T` argument tells `R` that any variable containing character strings should be interpreted as a qualitative variable, and that each distinct character string represents a distinct level for that qualitative variable. An easy way to load data from Excel into `R` is to save it as a csv (comma-separated values) file, and then use the `read.csv()` function.

```
> Auto <- read.csv("Auto.csv", na.strings = "?", stringsAsFactors =
    T)
> View(Auto)
```

[1] This function can sometimes be a bit finicky. If you have trouble using it, then try the `head()` function instead.

```
> dim(Auto)
[1] 397 9
> Auto[1:4, ]
```

The `dim()` function tells us that the data has 397 observations, or rows, and nine variables, or columns. There are various ways to deal with the missing data. In this case, only five of the rows contain missing observations, and so we choose to use the `na.omit()` function to simply remove these rows.

dim()

na.omit()

```
> Auto <- na.omit(Auto)
> dim(Auto)
[1] 392   9
```

Once the data are loaded correctly, we can use `names()` to check the variable names.

names()

```
> names(Auto)
[1] "mpg"          "cylinders"    "displacement" "horsepower"
[5] "weight"       "acceleration" "year"         "origin"
[9] "name"
```

2.3.5 Additional Graphical and Numerical Summaries

We can use the `plot()` function to produce *scatterplots* of the quantitative variables. However, simply typing the variable names will produce an error message, because `R` does not know to look in the `Auto` data set for those variables.

scatterplot

```
> plot(cylinders, mpg)
Error in plot(cylinders, mpg) : object `cylinders' not found
```

To refer to a variable, we must type the data set and the variable name joined with a `$` symbol. Alternatively, we can use the `attach()` function in order to tell `R` to make the variables in this data frame available by name.

attach()

```
> plot(Auto$cylinders, Auto$mpg)
> attach(Auto)
> plot(cylinders, mpg)
```

The `cylinders` variable is stored as a numeric vector, so `R` has treated it as quantitative. However, since there are only a small number of possible values for `cylinders`, one may prefer to treat it as a qualitative variable. The `as.factor()` function converts quantitative variables into qualitative variables.

as.factor()

```
> cylinders <- as.factor(cylinders)
```

If the variable plotted on the x-axis is qualitative, then *boxplots* will automatically be produced by the `plot()` function. As usual, a number of options can be specified in order to customize the plots.

boxplot

```
> plot(cylinders, mpg)
> plot(cylinders, mpg, col = "red")
> plot(cylinders, mpg, col = "red", varwidth = T)
```

```
> plot(cylinders, mpg, col = "red", varwidth = T,
    horizontal = T)
> plot(cylinders, mpg, col = "red", varwidth = T,
    xlab = "cylinders", ylab = "MPG")
```

The `hist()` function can be used to plot a *histogram*. Note that `col = 2` has the same effect as `col = "red"`.

`hist()`
histogram

```
> hist(mpg)
> hist(mpg, col = 2)
> hist(mpg, col = 2, breaks = 15)
```

The `pairs()` function creates a *scatterplot matrix*, i.e. a scatterplot for every pair of variables. We can also produce scatterplots for just a subset of the variables.

```
> pairs(Auto)
> pairs(
    ~ mpg + displacement + horsepower + weight + acceleration,
    data = Auto
  )
```

In conjunction with the `plot()` function, `identify()` provides a useful interactive method for identifying the value of a particular variable for points on a plot. We pass in three arguments to `identify()`: the x-axis variable, the y-axis variable, and the variable whose values we would like to see printed for each point. Then clicking one or more points in the plot and hitting Escape will cause `R` to print the values of the variable of interest. The numbers printed under the `identify()` function correspond to the rows for the selected points.

`identify()`

```
> plot(horsepower, mpg)
> identify(horsepower, mpg, name)
```

The `summary()` function produces a numerical summary of each variable in a particular data set.

`summary()`

```
> summary(Auto)
      mpg          cylinders      displacement
 Min.   : 9.00   Min.   :3.000   Min.   : 68.0
 1st Qu.:17.00   1st Qu.:4.000   1st Qu.:105.0
 Median :22.75   Median :4.000   Median :151.0
 Mean   :23.45   Mean   :5.472   Mean   :194.4
 3rd Qu.:29.00   3rd Qu.:8.000   3rd Qu.:275.8
 Max.   :46.60   Max.   :8.000   Max.   :455.0

   horsepower       weight      acceleration
 Min.   : 46.0   Min.   :1613   Min.   : 8.00
 1st Qu.: 75.0   1st Qu.:2225   1st Qu.:13.78
 Median : 93.5   Median :2804   Median :15.50
 Mean   :104.5   Mean   :2978   Mean   :15.54
 3rd Qu.:126.0   3rd Qu.:3615   3rd Qu.:17.02
 Max.   :230.0   Max.   :5140   Max.   :24.80

      year           origin                      name
```

```
Min.   :70.00   Min.   :1.000   amc matador       :  5
1st Qu.:73.00   1st Qu.:1.000   ford pinto        :  5
Median :76.00   Median :1.000   toyota corolla    :  5
Mean   :75.98   Mean   :1.577   amc gremlin       :  4
3rd Qu.:79.00   3rd Qu.:2.000   amc hornet        :  4
Max.   :82.00   Max.   :3.000   chevrolet chevette:  4
                                (Other)           :365
```

For qualitative variables such as `name`, `R` will list the number of observations that fall in each category. We can also produce a summary of just a single variable.

```
> summary(mpg)
   Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
   9.00   17.00   22.75   23.45   29.00   46.60
```

Once we have finished using `R`, we type `q()` in order to shut it down, or quit. When exiting `R`, we have the option to save the current *workspace* so that all objects (such as data sets) that we have created in this `R` session will be available next time. Before exiting `R`, we may want to save a record of all of the commands that we typed in the most recent session; this can be accomplished using the `savehistory()` function. Next time we enter `R`, we can load that history using the `loadhistory()` function, if we wish.

`q()`
workspace
`savehistory()`
`loadhistory()`

2.4 Exercises

Conceptual

1. For each of parts (a) through (d), indicate whether we would generally expect the performance of a flexible statistical learning method to be better or worse than an inflexible method. Justify your answer.

   (a) The sample size n is extremely large, and the number of predictors p is small.

   (b) The number of predictors p is extremely large, and the number of observations n is small.

   (c) The relationship between the predictors and response is highly non-linear.

   (d) The variance of the error terms, i.e. $\sigma^2 = \text{Var}(\epsilon)$, is extremely high.

2. Explain whether each scenario is a classification or regression problem, and indicate whether we are most interested in inference or prediction. Finally, provide n and p.

   (a) We collect a set of data on the top 500 firms in the US. For each firm we record profit, number of employees, industry and the CEO salary. We are interested in understanding which factors affect CEO salary.

(b) We are considering launching a new product and wish to know whether it will be a *success* or a *failure*. We collect data on 20 similar products that were previously launched. For each product we have recorded whether it was a success or failure, price charged for the product, marketing budget, competition price, and ten other variables.

(c) We are interested in predicting the % change in the USD/Euro exchange rate in relation to the weekly changes in the world stock markets. Hence we collect weekly data for all of 2012. For each week we record the % change in the USD/Euro, the % change in the US market, the % change in the British market, and the % change in the German market.

3. We now revisit the bias-variance decomposition.

(a) Provide a sketch of typical (squared) bias, variance, training error, test error, and Bayes (or irreducible) error curves, on a single plot, as we go from less flexible statistical learning methods towards more flexible approaches. The x-axis should represent the amount of flexibility in the method, and the y-axis should represent the values for each curve. There should be five curves. Make sure to label each one.

(b) Explain why each of the five curves has the shape displayed in part (a).

4. You will now think of some real-life applications for statistical learning.

(a) Describe three real-life applications in which *classification* might be useful. Describe the response, as well as the predictors. Is the goal of each application inference or prediction? Explain your answer.

(b) Describe three real-life applications in which *regression* might be useful. Describe the response, as well as the predictors. Is the goal of each application inference or prediction? Explain your answer.

(c) Describe three real-life applications in which *cluster analysis* might be useful.

5. What are the advantages and disadvantages of a very flexible (versus a less flexible) approach for regression or classification? Under what circumstances might a more flexible approach be preferred to a less flexible approach? When might a less flexible approach be preferred?

6. Describe the differences between a parametric and a non-parametric statistical learning approach. What are the advantages of a parametric approach to regression or classification (as opposed to a non-parametric approach)? What are its disadvantages?

7. The table below provides a training data set containing six observations, three predictors, and one qualitative response variable.

Obs.	X_1	X_2	X_3	Y
1	0	3	0	Red
2	2	0	0	Red
3	0	1	3	Red
4	0	1	2	Green
5	−1	0	1	Green
6	1	1	1	Red

Suppose we wish to use this data set to make a prediction for Y when $X_1 = X_2 = X_3 = 0$ using K-nearest neighbors.

(a) Compute the Euclidean distance between each observation and the test point, $X_1 = X_2 = X_3 = 0$.

(b) What is our prediction with $K = 1$? Why?

(c) What is our prediction with $K = 3$? Why?

(d) If the Bayes decision boundary in this problem is highly nonlinear, then would we expect the *best* value for K to be large or small? Why?

Applied

8. This exercise relates to the `College` data set, which can be found in the file `College.csv` on the book website. It contains a number of variables for 777 different universities and colleges in the US. The variables are

- `Private` : Public/private indicator
- `Apps` : Number of applications received
- `Accept` : Number of applicants accepted
- `Enroll` : Number of new students enrolled
- `Top10perc` : New students from top 10 % of high school class
- `Top25perc` : New students from top 25 % of high school class
- `F.Undergrad` : Number of full-time undergraduates
- `P.Undergrad` : Number of part-time undergraduates

- `Outstate` : Out-of-state tuition
- `Room.Board` : Room and board costs
- `Books` : Estimated book costs
- `Personal` : Estimated personal spending
- `PhD` : Percent of faculty with Ph.D.'s
- `Terminal` : Percent of faculty with terminal degree
- `S.F.Ratio` : Student/faculty ratio
- `perc.alumni` : Percent of alumni who donate
- `Expend` : Instructional expenditure per student
- `Grad.Rate` : Graduation rate

Before reading the data into `R`, it can be viewed in Excel or a text editor.

(a) Use the `read.csv()` function to read the data into `R`. Call the loaded data `college`. Make sure that you have the directory set to the correct location for the data.

(b) Look at the data using the `View()` function. You should notice that the first column is just the name of each university. We don't really want `R` to treat this as data. However, it may be handy to have these names for later. Try the following commands:

```
> rownames(college) <- college[, 1]
> View(college)
```

You should see that there is now a `row.names` column with the name of each university recorded. This means that `R` has given each row a name corresponding to the appropriate university. `R` will not try to perform calculations on the row names. However, we still need to eliminate the first column in the data where the names are stored. Try

```
> college <- college[, -1]
> View(college)
```

Now you should see that the first data column is `Private`. Note that another column labeled `row.names` now appears before the `Private` column. However, this is not a data column but rather the name that `R` is giving to each row.

(c) i. Use the `summary()` function to produce a numerical summary of the variables in the data set.

ii. Use the `pairs()` function to produce a scatterplot matrix of the first ten columns or variables of the data. Recall that you can reference the first ten columns of a matrix `A` using `A[,1:10]`.

iii. Use the `plot()` function to produce side-by-side boxplots of `Outstate` versus `Private`.

iv. Create a new qualitative variable, called `Elite`, by *binning* the `Top10perc` variable. We are going to divide universities into two groups based on whether or not the proportion of students coming from the top 10 % of their high school classes exceeds 50 %.

```
> Elite <- rep("No", nrow(college))
> Elite[college$Top10perc > 50] <- "Yes"
> Elite <- as.factor(Elite)
> college <- data.frame(college, Elite)
```

Use the `summary()` function to see how many elite universities there are. Now use the `plot()` function to produce side-by-side boxplots of `Outstate` versus `Elite`.

v. Use the `hist()` function to produce some histograms with differing numbers of bins for a few of the quantitative variables. You may find the command `par(mfrow = c(2, 2))` useful: it will divide the print window into four regions so that four plots can be made simultaneously. Modifying the arguments to this function will divide the screen in other ways.

vi. Continue exploring the data, and provide a brief summary of what you discover.

9. This exercise involves the `Auto` data set studied in the lab. Make sure that the missing values have been removed from the data.

(a) Which of the predictors are quantitative, and which are qualitative?

(b) What is the *range* of each quantitative predictor? You can answer this using the `range()` function.

`range()`

(c) What is the mean and standard deviation of each quantitative predictor?

(d) Now remove the 10th through 85th observations. What is the range, mean, and standard deviation of each predictor in the subset of the data that remains?

(e) Using the full data set, investigate the predictors graphically, using scatterplots or other tools of your choice. Create some plots highlighting the relationships among the predictors. Comment on your findings.

(f) Suppose that we wish to predict gas mileage (`mpg`) on the basis of the other variables. Do your plots suggest that any of the other variables might be useful in predicting `mpg`? Justify your answer.

10. This exercise involves the `Boston` housing data set.

    (a) To begin, load in the `Boston` data set. The `Boston` data set is part of the `ISLR2` *library*.

    ```
    > library(ISLR2)
    ```

    Now the data set is contained in the object `Boston`.

    ```
    > Boston
    ```

    Read about the data set:

    ```
    > ?Boston
    ```

    How many rows are in this data set? How many columns? What do the rows and columns represent?

    (b) Make some pairwise scatterplots of the predictors (columns) in this data set. Describe your findings.

    (c) Are any of the predictors associated with per capita crime rate? If so, explain the relationship.

    (d) Do any of the census tracts of Boston appear to have particularly high crime rates? Tax rates? Pupil-teacher ratios? Comment on the range of each predictor.

    (e) How many of the census tracts in this data set bound the Charles river?

    (f) What is the median pupil-teacher ratio among the towns in this data set?

    (g) Which census tract of Boston has lowest median value of owner-occupied homes? What are the values of the other predictors for that census tract, and how do those values compare to the overall ranges for those predictors? Comment on your findings.

    (h) In this data set, how many of the census tracts average more than seven rooms per dwelling? More than eight rooms per dwelling? Comment on the census tracts that average more than eight rooms per dwelling.

3

Linear Regression

This chapter is about *linear regression*, a very simple approach for supervised learning. In particular, linear regression is a useful tool for predicting a quantitative response. It has been around for a long time and is the topic of innumerable textbooks. Though it may seem somewhat dull compared to some of the more modern statistical learning approaches described in later chapters of this book, linear regression is still a useful and widely used statistical learning method. Moreover, it serves as a good jumping-off point for newer approaches: as we will see in later chapters, many fancy statistical learning approaches can be seen as generalizations or extensions of linear regression. Consequently, the importance of having a good understanding of linear regression before studying more complex learning methods cannot be overstated. In this chapter, we review some of the key ideas underlying the linear regression model, as well as the least squares approach that is most commonly used to fit this model.

Recall the `Advertising` data from Chapter 2. Figure 2.1 displays `sales` (in thousands of units) for a particular product as a function of advertising budgets (in thousands of dollars) for `TV`, `radio`, and `newspaper` media. Suppose that in our role as statistical consultants we are asked to suggest, on the basis of this data, a marketing plan for next year that will result in high product sales. What information would be useful in order to provide such a recommendation? Here are a few important questions that we might seek to address:

1. *Is there a relationship between advertising budget and sales?*
   Our first goal should be to determine whether the data provide evidence of an association between advertising expenditure and sales. If the evidence is weak, then one might argue that no money should be spent on advertising!

2. *How strong is the relationship between advertising budget and sales?*
   Assuming that there is a relationship between advertising and sales, we would like to know the strength of this relationship. Does knowledge of the advertising budget provide a lot of information about product sales?

3. *Which media are associated with sales?*
   Are all three media—TV, radio, and newspaper—associated with sales, or are just one or two of the media associated? To answer this question, we must find a way to separate out the individual contribution of each medium to sales when we have spent money on all three media.

4. *How large is the association between each medium and sales?*
   For every dollar spent on advertising in a particular medium, by what amount will sales increase? How accurately can we predict this amount of increase?

5. *How accurately can we predict future sales?*
   For any given level of television, radio, or newspaper advertising, what is our prediction for sales, and what is the accuracy of this prediction?

6. *Is the relationship linear?*
   If there is approximately a straight-line relationship between advertising expenditure in the various media and sales, then linear regression is an appropriate tool. If not, then it may still be possible to transform the predictor or the response so that linear regression can be used.

7. *Is there synergy among the advertising media?*
   Perhaps spending \$50,000 on television advertising and \$50,000 on radio advertising is associated with higher sales than allocating \$100,000 to either television or radio individually. In marketing, this is known as a *synergy* effect, while in statistics it is called an *interaction* effect.

synergy
interaction

It turns out that linear regression can be used to answer each of these questions. We will first discuss all of these questions in a general context, and then return to them in this specific context in Section 3.4.

3.1 Simple Linear Regression

Simple linear regression lives up to its name: it is a very straightforward approach for predicting a quantitative response Y on the basis of a single predictor variable X. It assumes that there is approximately a linear relationship between X and Y. Mathematically, we can write this linear relationship as

simple linear regression

$$Y \approx \beta_0 + \beta_1 X. \tag{3.1}$$

You might read "$\approx$" as *"is approximately modeled as"*. We will sometimes describe (3.1) by saying that we are *regressing* Y *on* X (or Y *onto* X). For example, X may represent `TV` advertising and Y may represent `sales`. Then we can regress `sales` onto `TV` by fitting the model

$$\texttt{sales} \approx \beta_0 + \beta_1 \times \texttt{TV}.$$

In Equation 3.1, β_0 and β_1 are two unknown constants that represent the *intercept* and *slope* terms in the linear model. Together, β_0 and β_1 are known as the model *coefficients* or *parameters*. Once we have used our training data to produce estimates $\hat{\beta}_0$ and $\hat{\beta}_1$ for the model coefficients, we can predict future sales on the basis of a particular value of TV advertising by computing

intercept
slope
coefficient
parameter

$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x, \tag{3.2}$$

where $\hat{y}$ indicates a prediction of Y on the basis of $X = x$. Here we use a *hat* symbol, $\hat{}$, to denote the estimated value for an unknown parameter or coefficient, or to denote the predicted value of the response.

3.1.1 Estimating the Coefficients

In practice, β_0 and β_1 are unknown. So before we can use (3.1) to make predictions, we must use data to estimate the coefficients. Let

$$(x_1, y_1),\ (x_2, y_2), \ldots,\ (x_n, y_n)$$

represent n observation pairs, each of which consists of a measurement of X and a measurement of Y. In the `Advertising` example, this data set consists of the TV advertising budget and product sales in $n = 200$ different markets. (Recall that the data are displayed in Figure 2.1.) Our goal is to obtain coefficient estimates $\hat{\beta}_0$ and $\hat{\beta}_1$ such that the linear model (3.1) fits the available data well—that is, so that $y_i \approx \hat{\beta}_0 + \hat{\beta}_1 x_i$ for $i = 1, \ldots, n$. In other words, we want to find an intercept $\hat{\beta}_0$ and a slope $\hat{\beta}_1$ such that the resulting line is as close as possible to the $n = 200$ data points. There are a number of ways of measuring *closeness*. However, by far the most common approach involves minimizing the *least squares* criterion, and we take that approach in this chapter. Alternative approaches will be considered in Chapter 6.

least squares

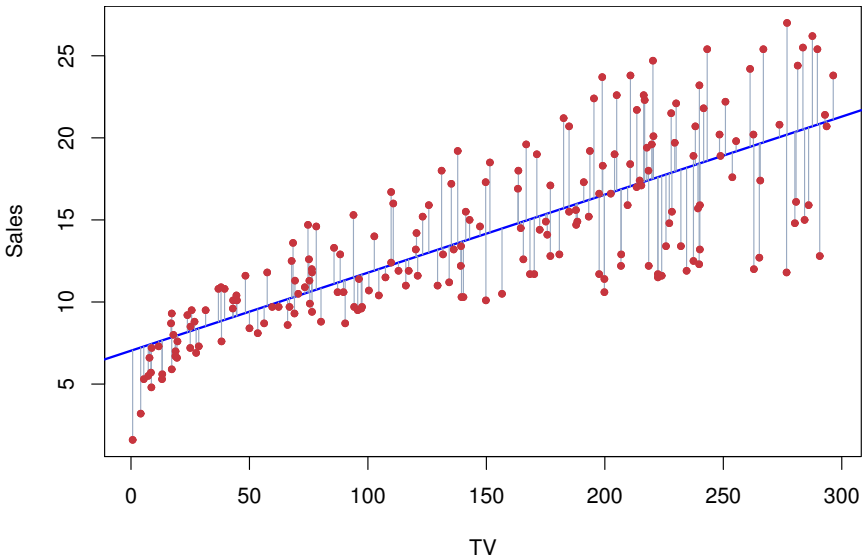


FIGURE 3.1. *For the* `Advertising` *data, the least squares fit for the regression of* `sales` *onto* `TV` *is shown. The fit is found by minimizing the residual sum of squares. Each grey line segment represents a residual. In this case a linear fit captures the essence of the relationship, although it overestimates the trend in the left of the plot.*

Let $\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i$ be the prediction for Y based on the ith value of X. Then $e_i = y_i - \hat{y}_i$ represents the ith *residual*—this is the difference between the ith observed response value and the ith response value that is predicted by our linear model. We define the *residual sum of squares* (RSS) as

residual

residual sum of squares

$$\text{RSS} = e_1^2 + e_2^2 + \cdots + e_n^2,$$

or equivalently as

$$\text{RSS} = (y_1 - \hat{\beta}_0 - \hat{\beta}_1 x_1)^2 + (y_2 - \hat{\beta}_0 - \hat{\beta}_1 x_2)^2 + \cdots + (y_n - \hat{\beta}_0 - \hat{\beta}_1 x_n)^2. \quad (3.3)$$

The least squares approach chooses $\hat{\beta}_0$ and $\hat{\beta}_1$ to minimize the RSS. Using some calculus, one can show that the minimizers are

$$\begin{aligned} \hat{\beta}_1 &= \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^n (x_i - \bar{x})^2}, \\ \hat{\beta}_0 &= \bar{y} - \hat{\beta}_1 \bar{x}, \end{aligned} \quad (3.4)$$

where $\bar{y} \equiv \frac{1}{n}\sum_{i=1}^n y_i$ and $\bar{x} \equiv \frac{1}{n}\sum_{i=1}^n x_i$ are the sample means. In other words, (3.4) defines the *least squares coefficient estimates* for simple linear regression.

Figure 3.1 displays the simple linear regression fit to the `Advertising` data, where $\hat{\beta}_0 = 7.03$ and $\hat{\beta}_1 = 0.0475$. In other words, according to

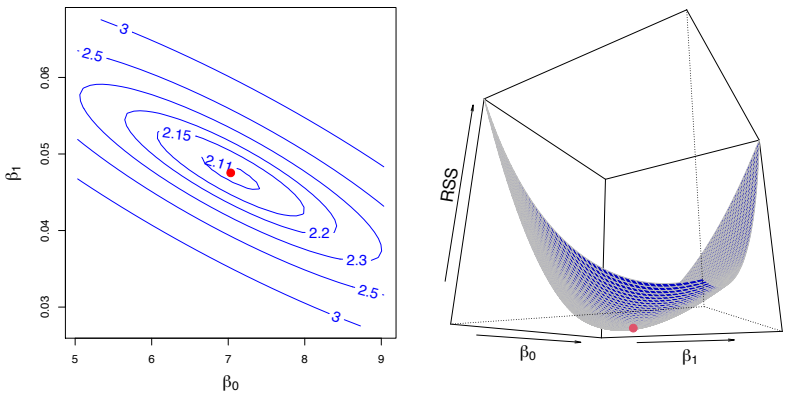


FIGURE 3.2. *Contour and three-dimensional plots of the RSS on the* `Advertising` *data, using* `sales` *as the response and* `TV` *as the predictor. The red dots correspond to the least squares estimates* $\hat{\beta}_0$ *and* $\hat{\beta}_1$*, given by (3.4).*

this approximation, an additional \$1,000 spent on TV advertising is associated with selling approximately 47.5 additional units of the product. In Figure 3.2, we have computed RSS for a number of values of β_0 and β_1, using the advertising data with `sales` as the response and `TV` as the predictor. In each plot, the red dot represents the pair of least squares estimates $(\hat{\beta}_0, \hat{\beta}_1)$ given by (3.4). These values clearly minimize the RSS.

3.1.2 Assessing the Accuracy of the Coefficient Estimates

Recall from (2.1) that we assume that the *true* relationship between X and Y takes the form $Y = f(X) + \epsilon$ for some unknown function f, where ϵ is a mean-zero random error term. If f is to be approximated by a linear function, then we can write this relationship as

$$Y = \beta_0 + \beta_1 X + \epsilon. \tag{3.5}$$

Here β_0 is the intercept term—that is, the expected value of Y when $X = 0$, and β_1 is the slope—the average increase in Y associated with a one-unit increase in X. The error term is a catch-all for what we miss with this simple model: the true relationship is probably not linear, there may be other variables that cause variation in Y, and there may be measurement error. We typically assume that the error term is independent of X.

The model given by (3.5) defines the *population regression line*, which is the best linear approximation to the true relationship between X and

population regression line

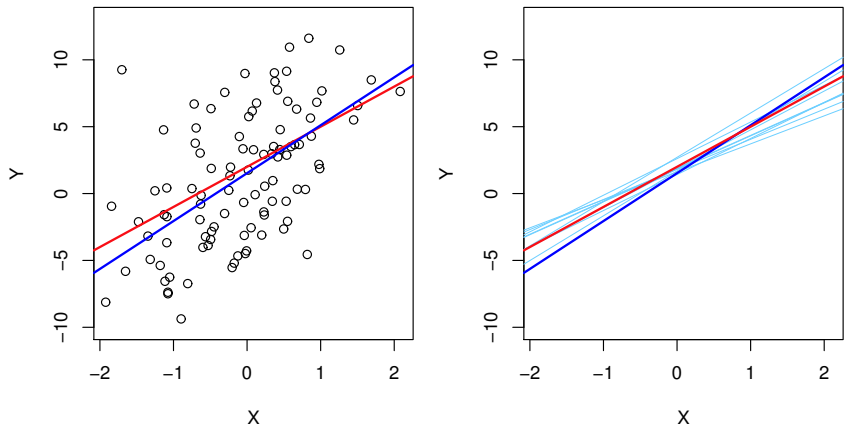


FIGURE 3.3. *A simulated data set.* Left: *The red line represents the true relationship,* $f(X) = 2 + 3X$*, which is known as the population regression line. The blue line is the least squares line; it is the least squares estimate for* $f(X)$ *based on the observed data, shown in black.* Right: *The population regression line is again shown in red, and the least squares line in dark blue. In light blue, ten least squares lines are shown, each computed on the basis of a separate random set of observations. Each least squares line is different, but on average, the least squares lines are quite close to the population regression line.*

Y.[1] The least squares regression coefficient estimates (3.4) characterize the *least squares line* (3.2). The left-hand panel of Figure 3.3 displays these two lines in a simple simulated example. We created 100 random Xs, and generated 100 corresponding Ys from the model

least squares line

$$Y = 2 + 3X + \epsilon, \tag{3.6}$$

where ϵ was generated from a normal distribution with mean zero. The red line in the left-hand panel of Figure 3.3 displays the *true* relationship, $f(X) = 2 + 3X$, while the blue line is the least squares estimate based on the observed data. The true relationship is generally not known for real data, but the least squares line can always be computed using the coefficient estimates given in (3.4). In other words, in real applications, we have access to a set of observations from which we can compute the least squares line; however, the population regression line is unobserved. In the right-hand panel of Figure 3.3 we have generated ten different data sets from the model given by (3.6) and plotted the corresponding ten least squares lines. Notice that different data sets generated from the same true model result in slightly different least squares lines, but the unobserved population regression line does not change.

[1]The assumption of linearity is often a useful working model. However, despite what many textbooks might tell us, we seldom believe that the true relationship is linear.

At first glance, the difference between the population regression line and the least squares line may seem subtle and confusing. We only have one data set, and so what does it mean that two different lines describe the relationship between the predictor and the response? Fundamentally, the concept of these two lines is a natural extension of the standard statistical approach of using information from a sample to estimate characteristics of a large population. For example, suppose that we are interested in knowing the population mean μ of some random variable Y. Unfortunately, μ is unknown, but we do have access to n observations from Y, $y_1, \ldots, y_n$, which we can use to estimate μ. A reasonable estimate is $\hat{\mu} = \bar{y}$, where $\bar{y} = \frac{1}{n}\sum_{i=1}^{n} y_i$ is the sample mean. The sample mean and the population mean are different, but in general the sample mean will provide a good estimate of the population mean. In the same way, the unknown coefficients β_0 and β_1 in linear regression define the population regression line. We seek to estimate these unknown coefficients using $\hat{\beta}_0$ and $\hat{\beta}_1$ given in (3.4). These coefficient estimates define the least squares line.

The analogy between linear regression and estimation of the mean of a random variable is an apt one based on the concept of *bias*. If we use the sample mean $\hat{\mu}$ to estimate μ, this estimate is *unbiased*, in the sense that on average, we expect $\hat{\mu}$ to equal μ. What exactly does this mean? It means that on the basis of one particular set of observations $y_1, \ldots, y_n$, $\hat{\mu}$ might overestimate μ, and on the basis of another set of observations, $\hat{\mu}$ might underestimate μ. But if we could average a huge number of estimates of μ obtained from a huge number of sets of observations, then this average would *exactly* equal μ. Hence, an unbiased estimator does not *systematically* over- or under-estimate the true parameter. The property of unbiasedness holds for the least squares coefficient estimates given by (3.4) as well: if we estimate β_0 and β_1 on the basis of a particular data set, then our estimates won't be exactly equal to β_0 and β_1. But if we could average the estimates obtained over a huge number of data sets, then the average of these estimates would be spot on! In fact, we can see from the right-hand panel of Figure 3.3 that the average of many least squares lines, each estimated from a separate data set, is pretty close to the true population regression line.

bias
unbiased

We continue the analogy with the estimation of the population mean μ of a random variable Y. A natural question is as follows: how accurate is the sample mean $\hat{\mu}$ as an estimate of μ? We have established that the average of $\hat{\mu}$'s over many data sets will be very close to μ, but that a single estimate $\hat{\mu}$ may be a substantial underestimate or overestimate of μ. How far off will that single estimate of $\hat{\mu}$ be? In general, we answer this question by computing the *standard error* of $\hat{\mu}$, written as $\mathrm{SE}(\hat{\mu})$. We have the well-known formula

standard error

$$\mathrm{Var}(\hat{\mu}) = \mathrm{SE}(\hat{\mu})^2 = \frac{\sigma^2}{n}, \tag{3.7}$$

where σ is the standard deviation of each of the realizations y_i of Y.[2] Roughly speaking, the standard error tells us the average amount that this estimate $\hat{\mu}$ differs from the actual value of μ. Equation 3.7 also tells us how this deviation shrinks with n—the more observations we have, the smaller the standard error of $\hat{\mu}$. In a similar vein, we can wonder how close $\hat{\beta}_0$ and $\hat{\beta}_1$ are to the true values β_0 and β_1. To compute the standard errors associated with $\hat{\beta}_0$ and $\hat{\beta}_1$, we use the following formulas:

$$\mathrm{SE}(\hat{\beta}_0)^2 = \sigma^2 \left[\frac{1}{n} + \frac{\bar{x}^2}{\sum_{i=1}^{n}(x_i - \bar{x})^2} \right], \quad \mathrm{SE}(\hat{\beta}_1)^2 = \frac{\sigma^2}{\sum_{i=1}^{n}(x_i - \bar{x})^2}, \quad (3.8)$$

where $\sigma^2 = \mathrm{Var}(\epsilon)$. For these formulas to be strictly valid, we need to assume that the errors ϵ_i for each observation have common variance σ^2 and are uncorrelated. This is clearly not true in Figure 3.1, but the formula still turns out to be a good approximation. Notice in the formula that $\mathrm{SE}(\hat{\beta}_1)$ is smaller when the x_i are more spread out; intuitively we have more *leverage* to estimate a slope when this is the case. We also see that $\mathrm{SE}(\hat{\beta}_0)$ would be the same as $\mathrm{SE}(\hat{\mu})$ if $\bar{x}$ were zero (in which case $\hat{\beta}_0$ would be equal to $\bar{y}$). In general, σ^2 is not known, but can be estimated from the data. This estimate of σ is known as the *residual standard error*, and is given by the formula $\mathrm{RSE} = \sqrt{\mathrm{RSS}/(n-2)}$. Strictly speaking, when σ^2 is estimated from the data we should write $\widehat{\mathrm{SE}}(\hat{\beta}_1)$ to indicate that an estimate has been made, but for simplicity of notation we will drop this extra "hat".

residual standard error

Standard errors can be used to compute *confidence intervals*. A 95 % confidence interval is defined as a range of values such that with 95 % probability, the range will contain the true unknown value of the parameter. The range is defined in terms of lower and upper limits computed from the sample of data. A 95% confidence interval has the following property: if we take repeated samples and construct the confidence interval for each sample, 95% of the intervals will contain the true unknown value of the parameter. For linear regression, the 95 % confidence interval for β_1 approximately takes the form

confidence interval

$$\hat{\beta}_1 \pm 2 \cdot \mathrm{SE}(\hat{\beta}_1). \quad (3.9)$$

That is, there is approximately a 95 % chance that the interval

$$\left[\hat{\beta}_1 - 2 \cdot \mathrm{SE}(\hat{\beta}_1),\ \hat{\beta}_1 + 2 \cdot \mathrm{SE}(\hat{\beta}_1) \right] \quad (3.10)$$

[2]This formula holds provided that the n observations are uncorrelated.

will contain the true value of β_1.[3] Similarly, a confidence interval for β_0 approximately takes the form

$$\hat{\beta}_0 \pm 2 \cdot \text{SE}(\hat{\beta}_0). \tag{3.11}$$

In the case of the advertising data, the 95 % confidence interval for β_0 is $[6.130, 7.935]$ and the 95 % confidence interval for β_1 is $[0.042, 0.053]$. Therefore, we can conclude that in the absence of any advertising, sales will, on average, fall somewhere between 6,130 and 7,935 units. Furthermore, for each $1,000 increase in television advertising, there will be an average increase in sales of between 42 and 53 units.

Standard errors can also be used to perform *hypothesis tests* on the coefficients. The most common hypothesis test involves testing the *null hypothesis* of

hypothesis test

null hypothesis

$$H_0 : \text{There is no relationship between } X \text{ and } Y \tag{3.12}$$

versus the *alternative hypothesis*

alternative hypothesis

$$H_a : \text{There is some relationship between } X \text{ and } Y. \tag{3.13}$$

Mathematically, this corresponds to testing

$$H_0 : \beta_1 = 0$$

versus

$$H_a : \beta_1 \neq 0,$$

since if $\beta_1 = 0$ then the model (3.5) reduces to $Y = \beta_0 + \epsilon$, and X is not associated with Y. To test the null hypothesis, we need to determine whether $\hat{\beta}_1$, our estimate for β_1, is sufficiently far from zero that we can be confident that β_1 is non-zero. How far is far enough? This of course depends on the accuracy of $\hat{\beta}_1$—that is, it depends on $\text{SE}(\hat{\beta}_1)$. If $\text{SE}(\hat{\beta}_1)$ is small, then even relatively small values of $\hat{\beta}_1$ may provide strong evidence that $\beta_1 \neq 0$, and hence that there is a relationship between X and Y. In contrast, if $\text{SE}(\hat{\beta}_1)$ is large, then $\hat{\beta}_1$ must be large in absolute value in order for us to reject the null hypothesis. In practice, we compute a *t-statistic*, given by

t-statistic

$$t = \frac{\hat{\beta}_1 - 0}{\text{SE}(\hat{\beta}_1)}, \tag{3.14}$$

[3] *Approximately* for several reasons. Equation 3.10 relies on the assumption that the errors are Gaussian. Also, the factor of 2 in front of the $\text{SE}(\hat{\beta}_1)$ term will vary slightly depending on the number of observations n in the linear regression. To be precise, rather than the number 2, (3.10) should contain the 97.5 % quantile of a t-distribution with $n-2$ degrees of freedom. Details of how to compute the 95 % confidence interval precisely in R will be provided later in this chapter.

	Coefficient	Std. error	t-statistic	p-value
Intercept	7.0325	0.4578	15.36	< 0.0001
TV	0.0475	0.0027	17.67	< 0.0001

TABLE 3.1. *For the* Advertising *data, coefficients of the least squares model for the regression of number of units sold on TV advertising budget. An increase of* \$1,000 *in the TV advertising budget is associated with an increase in sales by around 50 units. (Recall that the* sales *variable is in thousands of units, and the* TV *variable is in thousands of dollars.)*

which measures the number of standard deviations that $\hat{\beta}_1$ is away from 0. If there really is no relationship between X and Y, then we expect that (3.14) will have a t-distribution with $n-2$ degrees of freedom. The t-distribution has a bell shape and for values of n greater than approximately 30 it is quite similar to the standard normal distribution. Consequently, it is a simple matter to compute the probability of observing any number equal to $|t|$ or larger in absolute value, assuming $\beta_1 = 0$. We call this probability the *p-value*. Roughly speaking, we interpret the p-value as follows: a small p-value indicates that it is unlikely to observe such a substantial association between the predictor and the response due to chance, in the absence of any real association between the predictor and the response. Hence, if we see a small p-value, then we can infer that there is an association between the predictor and the response. We *reject the null hypothesis*—that is, we declare a relationship to exist between X and Y—if the p-value is small enough. Typical p-value cutoffs for rejecting the null hypothesis are 5% or 1%, although this topic will be explored in much greater detail in Chapter 13. When $n = 30$, these correspond to t-statistics (3.14) of around 2 and 2.75, respectively.

p-value

Table 3.1 provides details of the least squares model for the regression of number of units sold on TV advertising budget for the Advertising data. Notice that the coefficients for $\hat{\beta}_0$ and $\hat{\beta}_1$ are very large relative to their standard errors, so the t-statistics are also large; the probabilities of seeing such values if H_0 is true are virtually zero. Hence we can conclude that $\beta_0 \neq 0$ and $\beta_1 \neq 0$.[4]

3.1.3 Assessing the Accuracy of the Model

Once we have rejected the null hypothesis (3.12) in favor of the alternative hypothesis (3.13), it is natural to want to quantify *the extent to which the model fits the data*. The quality of a linear regression fit is typically assessed

[4]In Table 3.1, a small p-value for the intercept indicates that we can reject the null hypothesis that $\beta_0 = 0$, and a small p-value for TV indicates that we can reject the null hypothesis that $\beta_1 = 0$. Rejecting the latter null hypothesis allows us to conclude that there is a relationship between TV and sales. Rejecting the former allows us to conclude that in the absence of TV expenditure, sales are non-zero.

Quantity	Value
Residual standard error	3.26
R^2	0.612
F-statistic	312.1

TABLE 3.2. *For the* `Advertising` *data, more information about the least squares model for the regression of number of units sold on TV advertising budget.*

using two related quantities: the *residual standard error* (RSE) and the R^2 statistic. R^2

Table 3.2 displays the RSE, the R^2 statistic, and the F-statistic (to be described in Section 3.2.2) for the linear regression of number of units sold on TV advertising budget.

Residual Standard Error

Recall from the model (3.5) that associated with each observation is an error term ϵ. Due to the presence of these error terms, even if we knew the true regression line (i.e. even if β_0 and β_1 were known), we would not be able to perfectly predict Y from X. The RSE is an estimate of the standard deviation of ϵ. Roughly speaking, it is the average amount that the response will deviate from the true regression line. It is computed using the formula

$$\text{RSE} = \sqrt{\frac{1}{n-2}\text{RSS}} = \sqrt{\frac{1}{n-2}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}. \tag{3.15}$$

Note that RSS was defined in Section 3.1.1, and is given by the formula

$$\text{RSS} = \sum_{i=1}^{n}(y_i - \hat{y}_i)^2. \tag{3.16}$$

In the case of the advertising data, we see from the linear regression output in Table 3.2 that the RSE is 3.26. In other words, actual sales in each market deviate from the true regression line by approximately 3,260 units, on average. Another way to think about this is that even if the model were correct and the true values of the unknown coefficients β_0 and β_1 were known exactly, any prediction of sales on the basis of TV advertising would still be off by about 3,260 units on average. Of course, whether or not 3,260 units is an acceptable prediction error depends on the problem context. In the advertising data set, the mean value of `sales` over all markets is approximately 14,000 units, and so the percentage error is 3,260/14,000 = 23 %.

The RSE is considered a measure of the *lack of fit* of the model (3.5) to the data. If the predictions obtained using the model are very close to the true outcome values—that is, if $\hat{y}_i \approx y_i$ for $i = 1, \ldots, n$—then (3.15) will be small, and we can conclude that the model fits the data very well. On

the other hand, if $\hat{y}_i$ is very far from y_i for one or more observations, then the RSE may be quite large, indicating that the model doesn't fit the data well.

R^2 Statistic

The RSE provides an absolute measure of lack of fit of the model (3.5) to the data. But since it is measured in the units of Y, it is not always clear what constitutes a good RSE. The R^2 statistic provides an alternative measure of fit. It takes the form of a *proportion*—the proportion of variance explained—and so it always takes on a value between 0 and 1, and is independent of the scale of Y.

To calculate R^2, we use the formula

$$R^2 = \frac{\text{TSS} - \text{RSS}}{\text{TSS}} = 1 - \frac{\text{RSS}}{\text{TSS}} \tag{3.17}$$

where $\text{TSS} = \sum(y_i - \bar{y})^2$ is the *total sum of squares*, and RSS is defined in (3.16). TSS measures the total variance in the response Y, and can be thought of as the amount of variability inherent in the response before the regression is performed. In contrast, RSS measures the amount of variability that is left unexplained after performing the regression. Hence, $\text{TSS} - \text{RSS}$ measures the amount of variability in the response that is explained (or removed) by performing the regression, and R^2 measures the *proportion of variability in* Y *that can be explained using* X. An R^2 statistic that is close to 1 indicates that a large proportion of the variability in the response is explained by the regression. A number near 0 indicates that the regression does not explain much of the variability in the response; this might occur because the linear model is wrong, or the error variance σ^2 is high, or both. In Table 3.2, the R^2 was 0.61, and so just under two-thirds of the variability in `sales` is explained by a linear regression on `TV`.

total sum of squares

The R^2 statistic (3.17) has an interpretational advantage over the RSE (3.15), since unlike the RSE, it always lies between 0 and 1. However, it can still be challenging to determine what is a *good* R^2 value, and in general, this will depend on the application. For instance, in certain problems in physics, we may know that the data truly comes from a linear model with a small residual error. In this case, we would expect to see an R^2 value that is extremely close to 1, and a substantially smaller R^2 value might indicate a serious problem with the experiment in which the data were generated. On the other hand, in typical applications in biology, psychology, marketing, and other domains, the linear model (3.5) is at best an extremely rough approximation to the data, and residual errors due to other unmeasured factors are often very large. In this setting, we would expect only a very small proportion of the variance in the response to be explained by the predictor, and an R^2 value well below 0.1 might be more realistic!

The R^2 statistic is a measure of the linear relationship between X and Y. Recall that *correlation*, defined as

correlation

$$\text{Cor}(X, Y) = \frac{\sum_{i=1}^{n}(x_i - \overline{x})(y_i - \overline{y})}{\sqrt{\sum_{i=1}^{n}(x_i - \overline{x})^2}\sqrt{\sum_{i=1}^{n}(y_i - \overline{y})^2}}, \tag{3.18}$$

is also a measure of the linear relationship between X and Y.[5] This suggests that we might be able to use $r = \text{Cor}(X, Y)$ instead of R^2 in order to assess the fit of the linear model. In fact, it can be shown that in the simple linear regression setting, $R^2 = r^2$. In other words, the squared correlation and the R^2 statistic are identical. However, in the next section we will discuss the multiple linear regression problem, in which we use several predictors simultaneously to predict the response. The concept of correlation between the predictors and the response does not extend automatically to this setting, since correlation quantifies the association between a single pair of variables rather than between a larger number of variables. We will see that R^2 fills this role.

3.2 Multiple Linear Regression

Simple linear regression is a useful approach for predicting a response on the basis of a single predictor variable. However, in practice we often have more than one predictor. For example, in the `Advertising` data, we have examined the relationship between sales and TV advertising. We also have data for the amount of money spent advertising on the radio and in newspapers, and we may want to know whether either of these two media is associated with sales. How can we extend our analysis of the advertising data in order to accommodate these two additional predictors?

One option is to run three separate simple linear regressions, each of which uses a different advertising medium as a predictor. For instance, we can fit a simple linear regression to predict sales on the basis of the amount spent on radio advertisements. Results are shown in Table 3.3 (top table). We find that a \$1,000 increase in spending on radio advertising is associated with an increase in sales of around 203 units. Table 3.3 (bottom table) contains the least squares coefficients for a simple linear regression of sales onto newspaper advertising budget. A \$1,000 increase in newspaper advertising budget is associated with an increase in sales of approximately 55 units.

However, the approach of fitting a separate simple linear regression model for each predictor is not entirely satisfactory. First of all, it is unclear how to make a single prediction of sales given the three advertising media budgets, since each of the budgets is associated with a separate regression equation.

[5] We note that in fact, the right-hand side of (3.18) is the sample correlation; thus, it would be more correct to write $\widehat{\text{Cor}}(X, Y)$; however, we omit the "hat" for ease of notation.

Simple regression of sales on radio

	Coefficient	Std. error	t-statistic	p-value
Intercept	9.312	0.563	16.54	< 0.0001
radio	0.203	0.020	9.92	< 0.0001

Simple regression of sales on newspaper

	Coefficient	Std. error	t-statistic	p-value
Intercept	12.351	0.621	19.88	< 0.0001
newspaper	0.055	0.017	3.30	0.00115

TABLE 3.3. *More simple linear regression models for the* Advertising *data. Coefficients of the simple linear regression model for number of units sold on* Top: *radio advertising budget and* Bottom: *newspaper advertising budget. A* \$1,000 *increase in spending on radio advertising is associated with an average increase in sales by around 203 units, while the same increase in spending on newspaper advertising is associated with an average increase in sales by around 55 units. (Note that the* sales *variable is in thousands of units, and the* radio *and* newspaper *variables are in thousands of dollars.)*

Second, each of the three regression equations ignores the other two media in forming estimates for the regression coefficients. We will see shortly that if the media budgets are correlated with each other in the 200 markets in our data set, then this can lead to very misleading estimates of the association between each media budget and sales.

Instead of fitting a separate simple linear regression model for each predictor, a better approach is to extend the simple linear regression model (3.5) so that it can directly accommodate multiple predictors. We can do this by giving each predictor a separate slope coefficient in a single model. In general, suppose that we have p distinct predictors. Then the multiple linear regression model takes the form

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_p X_p + \epsilon, \tag{3.19}$$

where X_j represents the jth predictor and β_j quantifies the association between that variable and the response. We interpret β_j as the *average* effect on Y of a one unit increase in X_j, *holding all other predictors fixed*. In the advertising example, (3.19) becomes

$$\texttt{sales} = \beta_0 + \beta_1 \times \texttt{TV} + \beta_2 \times \texttt{radio} + \beta_3 \times \texttt{newspaper} + \epsilon. \tag{3.20}$$

3.2.1 Estimating the Regression Coefficients

As was the case in the simple linear regression setting, the regression coefficients $\beta_0, \beta_1, \ldots, \beta_p$ in (3.19) are unknown, and must be estimated. Given

estimates $\hat{\beta}_0, \hat{\beta}_1, \ldots, \hat{\beta}_p$, we can make predictions using the formula

$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2 + \cdots + \hat{\beta}_p x_p. \tag{3.21}$$

The parameters are estimated using the same least squares approach that we saw in the context of simple linear regression. We choose $\beta_0, \beta_1, \ldots, \beta_p$ to minimize the sum of squared residuals

$$\begin{aligned} \text{RSS} &= \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 \\ &= \sum_{i=1}^{n} (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_{i1} - \hat{\beta}_2 x_{i2} - \cdots - \hat{\beta}_p x_{ip})^2. \end{aligned} \tag{3.22}$$

The values $\hat{\beta}_0, \hat{\beta}_1, \ldots, \hat{\beta}_p$ that minimize (3.22) are the multiple least squares regression coefficient estimates. Unlike the simple linear regression estimates given in (3.4), the multiple regression coefficient estimates have somewhat complicated forms that are most easily represented using matrix algebra. For this reason, we do not provide them here. Any statistical software package can be used to compute these coefficient estimates, and later in this chapter we will show how this can be done in R. Figure 3.4 illustrates an example of the least squares fit to a toy data set with $p = 2$ predictors.

Table 3.4 displays the multiple regression coefficient estimates when TV, radio, and newspaper advertising budgets are used to predict product sales using the Advertising data. We interpret these results as follows: for a given amount of TV and newspaper advertising, spending an additional $1,000 on radio advertising is associated with approximately 189 units of additional sales. Comparing these coefficient estimates to those displayed in Tables 3.1 and 3.3, we notice that the multiple regression coefficient estimates for TV and radio are pretty similar to the simple linear regression coefficient estimates. However, while the newspaper regression coefficient estimate in Table 3.3 was significantly non-zero, the coefficient estimate for newspaper in the multiple regression model is close to zero, and the corresponding p-value is no longer significant, with a value around 0.86. This illustrates that the simple and multiple regression coefficients can be quite different. This difference stems from the fact that in the simple regression case, the slope term represents the average increase in product sales associated with a $1,000 increase in newspaper advertising, ignoring other predictors such as TV and radio. By contrast, in the multiple regression setting, the coefficient for newspaper represents the average increase in product sales associated with increasing newspaper spending by $1,000 while holding TV and radio fixed.

Does it make sense for the multiple regression to suggest no relationship between sales and newspaper while the simple linear regression implies the

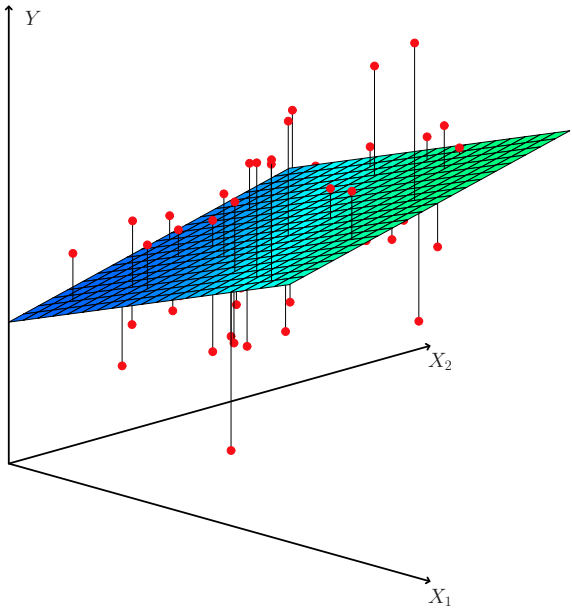


FIGURE 3.4. *In a three-dimensional setting, with two predictors and one response, the least squares regression line becomes a plane. The plane is chosen to minimize the sum of the squared vertical distances between each observation (shown in red) and the plane.*

opposite? In fact it does. Consider the correlation matrix for the three predictor variables and response variable, displayed in Table 3.5. Notice that the correlation between `radio` and `newspaper` is 0.35. This indicates that markets with high newspaper advertising tend to also have high radio advertising. Now suppose that the multiple regression is correct and newspaper advertising is not associated with sales, but radio advertising is associated with sales. Then in markets where we spend more on radio our sales will tend to be higher, and as our correlation matrix shows, we also tend to spend more on newspaper advertising in those same markets. Hence, in a simple linear regression which only examines `sales` versus

	Coefficient	Std. error	t-statistic	p-value
`Intercept`	2.939	0.3119	9.42	< 0.0001
`TV`	0.046	0.0014	32.81	< 0.0001
`radio`	0.189	0.0086	21.89	< 0.0001
`newspaper`	−0.001	0.0059	−0.18	0.8599

TABLE 3.4. *For the* `Advertising` *data, least squares coefficient estimates of the multiple linear regression of number of units sold on TV, radio, and newspaper advertising budgets.*

	TV	radio	newspaper	sales
TV	1.0000	0.0548	0.0567	0.7822
radio		1.0000	0.3541	0.5762
newspaper			1.0000	0.2283
sales				1.0000

TABLE 3.5. *Correlation matrix for* TV, radio, newspaper, *and* sales *for the* Advertising *data.*

newspaper, we will observe that higher values of newspaper tend to be associated with higher values of sales, even though newspaper advertising is not directly associated with sales. So newspaper advertising is a surrogate for radio advertising; newspaper gets "credit" for the association between radio on sales.

This slightly counterintuitive result is very common in many real life situations. Consider an absurd example to illustrate the point. Running a regression of shark attacks versus ice cream sales for data collected at a given beach community over a period of time would show a positive relationship, similar to that seen between sales and newspaper. Of course no one has (yet) suggested that ice creams should be banned at beaches to reduce shark attacks. In reality, higher temperatures cause more people to visit the beach, which in turn results in more ice cream sales and more shark attacks. A multiple regression of shark attacks onto ice cream sales and temperature reveals that, as intuition implies, ice cream sales is no longer a significant predictor after adjusting for temperature.

3.2.2 Some Important Questions

When we perform multiple linear regression, we usually are interested in answering a few important questions.

1. *Is at least one of the predictors $X_1, X_2, \ldots, X_p$ useful in predicting the response?*
2. *Do all the predictors help to explain Y, or is only a subset of the predictors useful?*
3. *How well does the model fit the data?*
4. *Given a set of predictor values, what response value should we predict, and how accurate is our prediction?*

We now address each of these questions in turn.

One: Is There a Relationship Between the Response and Predictors?

Recall that in the simple linear regression setting, in order to determine whether there is a relationship between the response and the predictor we

Quantity	Value
Residual standard error	1.69
R^2	0.897
F-statistic	570

TABLE 3.6. *More information about the least squares model for the regression of number of units sold on TV, newspaper, and radio advertising budgets in the* `Advertising` *data. Other information about this model was displayed in Table 3.4.*

can simply check whether $\beta_1 = 0$. In the multiple regression setting with p predictors, we need to ask whether all of the regression coefficients are zero, i.e. whether $\beta_1 = \beta_2 = \cdots = \beta_p = 0$. As in the simple linear regression setting, we use a hypothesis test to answer this question. We test the null hypothesis,

$$H_0 : \beta_1 = \beta_2 = \cdots = \beta_p = 0$$

versus the alternative

$$H_a : \text{ at least one } \beta_j \text{ is non-zero.}$$

This hypothesis test is performed by computing the *F-statistic*,

F-statistic

$$F = \frac{(\text{TSS} - \text{RSS})/p}{\text{RSS}/(n-p-1)}, \tag{3.23}$$

where, as with simple linear regression, $\text{TSS} = \sum(y_i - \bar{y})^2$ and $\text{RSS} = \sum(y_i - \hat{y}_i)^2$. If the linear model assumptions are correct, one can show that

$$E\{\text{RSS}/(n-p-1)\} = \sigma^2$$

and that, provided H_0 is true,

$$E\{(\text{TSS} - \text{RSS})/p\} = \sigma^2.$$

Hence, when there is no relationship between the response and predictors, one would expect the F-statistic to take on a value close to 1. On the other hand, if H_a is true, then $E\{(\text{TSS} - \text{RSS})/p\} > \sigma^2$, so we expect F to be greater than 1.

The F-statistic for the multiple linear regression model obtained by regressing `sales` onto `radio`, `TV`, and `newspaper` is shown in Table 3.6. In this example the F-statistic is 570. Since this is far larger than 1, it provides compelling evidence against the null hypothesis H_0. In other words, the large F-statistic suggests that at least one of the advertising media must be related to `sales`. However, what if the F-statistic had been closer to 1? How large does the F-statistic need to be before we can reject H_0 and conclude that there is a relationship? It turns out that the answer depends on the values of n and p. When n is large, an F-statistic that is just a little larger than 1 might still provide evidence against H_0. In contrast,

a larger F-statistic is needed to reject H_0 if n is small. When H_0 is true and the errors ϵ_i have a normal distribution, the F-statistic follows an F-distribution.[6] For any given value of n and p, any statistical software package can be used to compute the p-value associated with the F-statistic using this distribution. Based on this p-value, we can determine whether or not to reject H_0. For the advertising data, the p-value associated with the F-statistic in Table 3.6 is essentially zero, so we have extremely strong evidence that at least one of the media is associated with increased `sales`.

In (3.23) we are testing H_0 that all the coefficients are zero. Sometimes we want to test that a particular subset of q of the coefficients are zero. This corresponds to a null hypothesis

$$H_0 : \quad \beta_{p-q+1} = \beta_{p-q+2} = \cdots = \beta_p = 0,$$

where for convenience we have put the variables chosen for omission at the end of the list. In this case we fit a second model that uses all the variables *except* those last q. Suppose that the residual sum of squares for that model is RSS_0. Then the appropriate F-statistic is

$$F = \frac{(\text{RSS}_0 - \text{RSS})/q}{\text{RSS}/(n-p-1)}. \tag{3.24}$$

Notice that in Table 3.4, for each individual predictor a t-statistic and a p-value were reported. These provide information about whether each individual predictor is related to the response, after adjusting for the other predictors. It turns out that each of these is exactly equivalent[7] to the F-test that omits that single variable from the model, leaving all the others in—i.e. q=1 in (3.24). So it reports the *partial effect* of adding that variable to the model. For instance, as we discussed earlier, these p-values indicate that `TV` and `radio` are related to `sales`, but that there is no evidence that `newspaper` is associated with `sales`, when `TV` and `radio` are held fixed.

Given these individual p-values for each variable, why do we need to look at the overall F-statistic? After all, it seems likely that if any one of the p-values for the individual variables is very small, then *at least one of the predictors is related to the response*. However, this logic is flawed, especially when the number of predictors p is large.

For instance, consider an example in which $p = 100$ and $H_0 : \beta_1 = \beta_2 = \cdots = \beta_p = 0$ is true, so no variable is truly associated with the response. In this situation, about 5 % of the p-values associated with each variable (of the type shown in Table 3.4) will be below 0.05 by chance. In other words, we expect to see approximately five *small* p-values even in the absence of

[6] Even if the errors are not normally-distributed, the F-statistic approximately follows an F-distribution provided that the sample size n is large.

[7] The square of each t-statistic is the corresponding F-statistic.

any true association between the predictors and the response.[8] In fact, it is likely that we will observe at least one p-value below 0.05 by chance! Hence, if we use the individual t-statistics and associated p-values in order to decide whether or not there is any association between the variables and the response, there is a very high chance that we will incorrectly conclude that there is a relationship. However, the F-statistic does not suffer from this problem because it adjusts for the number of predictors. Hence, if H_0 is true, there is only a 5 % chance that the F-statistic will result in a p-value below 0.05, regardless of the number of predictors or the number of observations.

The approach of using an F-statistic to test for any association between the predictors and the response works when p is relatively small, and certainly small compared to n. However, sometimes we have a very large number of variables. If $p > n$ then there are more coefficients β_j to estimate than observations from which to estimate them. In this case we cannot even fit the multiple linear regression model using least squares, so the F-statistic cannot be used, and neither can most of the other concepts that we have seen so far in this chapter. When p is large, some of the approaches discussed in the next section, such as *forward selection*, can be used. This *high-dimensional* setting is discussed in greater detail in Chapter 6.

high-dimensional

Two: Deciding on Important Variables

As discussed in the previous section, the first step in a multiple regression analysis is to compute the F-statistic and to examine the associated p-value. If we conclude on the basis of that p-value that at least one of the predictors is related to the response, then it is natural to wonder *which* are the guilty ones! We could look at the individual p-values as in Table 3.4, but as discussed (and as further explored in Chapter 13), if p is large we are likely to make some false discoveries.

It is possible that all of the predictors are associated with the response, but it is more often the case that the response is only associated with a subset of the predictors. The task of determining which predictors are associated with the response, in order to fit a single model involving only those predictors, is referred to as *variable selection*. The variable selection problem is studied extensively in Chapter 6, and so here we will provide only a brief outline of some classical approaches.

variable selection

Ideally, we would like to perform variable selection by trying out a lot of different models, each containing a different subset of the predictors. For instance, if $p = 2$, then we can consider four models: (1) a model containing no variables, (2) a model containing X_1 only, (3) a model containing X_2 only, and (4) a model containing both X_1 and X_2. We can then se-

[8] This is related to the important concept of *multiple testing*, which is the focus of Chapter 13.

lect the *best* model out of all of the models that we have considered. How do we determine which model is best? Various statistics can be used to judge the quality of a model. These include *Mallow's* C_p, *Akaike information criterion* (AIC), *Bayesian information criterion* (BIC), and *adjusted* R^2. These are discussed in more detail in Chapter 6. We can also determine which model is best by plotting various model outputs, such as the residuals, in order to search for patterns.

Mallow's C_p
Akaike information criterion
Bayesian information criterion
adjusted R^2

Unfortunately, there are a total of 2^p models that contain subsets of p variables. This means that even for moderate p, trying out every possible subset of the predictors is infeasible. For instance, we saw that if $p = 2$, then there are $2^2 = 4$ models to consider. But if $p = 30$, then we must consider $2^{30} = 1{,}073{,}741{,}824$ models! This is not practical. Therefore, unless p is very small, we cannot consider all 2^p models, and instead we need an automated and efficient approach to choose a smaller set of models to consider. There are three classical approaches for this task:

- *Forward selection*. We begin with the *null model*—a model that contains an intercept but no predictors. We then fit p simple linear regressions and add to the null model the variable that results in the lowest RSS. We then add to that model the variable that results in the lowest RSS for the new two-variable model. This approach is continued until some stopping rule is satisfied.

forward selection
null model

- *Backward selection*. We start with all variables in the model, and remove the variable with the largest p-value—that is, the variable that is the least statistically significant. The new $(p-1)$-variable model is fit, and the variable with the largest p-value is removed. This procedure continues until a stopping rule is reached. For instance, we may stop when all remaining variables have a p-value below some threshold.

backward selection

- *Mixed selection*. This is a combination of forward and backward selection. We start with no variables in the model, and as with forward selection, we add the variable that provides the best fit. We continue to add variables one-by-one. Of course, as we noted with the `Advertising` example, the p-values for variables can become larger as new predictors are added to the model. Hence, if at any point the p-value for one of the variables in the model rises above a certain threshold, then we remove that variable from the model. We continue to perform these forward and backward steps until all variables in the model have a sufficiently low p-value, and all variables outside the model would have a large p-value if added to the model.

mixed selection

Backward selection cannot be used if $p > n$, while forward selection can always be used. Forward selection is a greedy approach, and might include variables early that later become redundant. Mixed selection can remedy this.

Three: Model Fit

Two of the most common numerical measures of model fit are the RSE and R^2, the fraction of variance explained. These quantities are computed and interpreted in the same fashion as for simple linear regression.

Recall that in simple regression, R^2 is the square of the correlation of the response and the variable. In multiple linear regression, it turns out that it equals $\text{Cor}(Y, \hat{Y})^2$, the square of the correlation between the response and the fitted linear model; in fact one property of the fitted linear model is that it maximizes this correlation among all possible linear models.

An R^2 value close to 1 indicates that the model explains a large portion of the variance in the response variable. As an example, we saw in Table 3.6 that for the `Advertising` data, the model that uses all three advertising media to predict `sales` has an R^2 of 0.8972. On the other hand, the model that uses only `TV` and `radio` to predict `sales` has an R^2 value of 0.89719. In other words, there is a *small* increase in R^2 if we include newspaper advertising in the model that already contains TV and radio advertising, even though we saw earlier that the p-value for newspaper advertising in Table 3.4 is not significant. It turns out that R^2 will always increase when more variables are added to the model, even if those variables are only weakly associated with the response. This is due to the fact that adding another variable always results in a decrease in the residual sum of squares on the training data (though not necessarily the testing data). Thus, the R^2 statistic, which is also computed on the training data, must increase. The fact that adding newspaper advertising to the model containing only TV and radio advertising leads to just a tiny increase in R^2 provides additional evidence that `newspaper` can be dropped from the model. Essentially, `newspaper` provides no real improvement in the model fit to the training samples, and its inclusion will likely lead to poor results on independent test samples due to overfitting.

By contrast, the model containing only `TV` as a predictor had an R^2 of 0.61 (Table 3.2). Adding `radio` to the model leads to a substantial improvement in R^2. This implies that a model that uses TV and radio expenditures to predict sales is substantially better than one that uses only TV advertising. We could further quantify this improvement by looking at the p-value for the `radio` coefficient in a model that contains only `TV` and `radio` as predictors.

The model that contains only `TV` and `radio` as predictors has an RSE of 1.681, and the model that also contains `newspaper` as a predictor has an RSE of 1.686 (Table 3.6). In contrast, the model that contains only `TV` has an RSE of 3.26 (Table 3.2). This corroborates our previous conclusion that a model that uses TV and radio expenditures to predict sales is much more accurate (on the training data) than one that only uses TV spending. Furthermore, given that TV and radio expenditures are used as predictors, there is no point in also using newspaper spending as a predictor in the

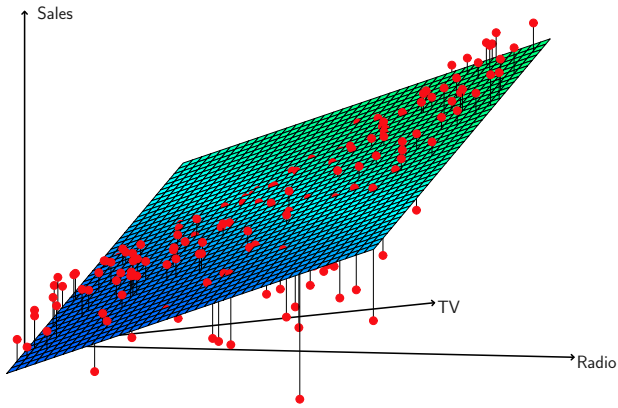


FIGURE 3.5. *For the* `Advertising` *data, a linear regression fit to* `sales` *using* `TV` *and* `radio` *as predictors. From the pattern of the residuals, we can see that there is a pronounced non-linear relationship in the data. The positive residuals (those visible above the surface), tend to lie along the 45-degree line, where TV and Radio budgets are split evenly. The negative residuals (most not visible), tend to lie away from this line, where budgets are more lopsided.*

model. The observant reader may wonder how RSE can increase when `newspaper` is added to the model given that RSS must decrease. In general RSE is defined as

$$\text{RSE} = \sqrt{\frac{1}{n-p-1}\text{RSS}}, \tag{3.25}$$

which simplifies to (3.15) for a simple linear regression. Thus, models with more variables can have higher RSE if the decrease in RSS is small relative to the increase in p.

In addition to looking at the RSE and R^2 statistics just discussed, it can be useful to plot the data. Graphical summaries can reveal problems with a model that are not visible from numerical statistics. For example, Figure 3.5 displays a three-dimensional plot of `TV` and `radio` versus `sales`. We see that some observations lie above and some observations lie below the least squares regression plane. In particular, the linear model seems to overestimate `sales` for instances in which most of the advertising money was spent exclusively on either `TV` or `radio`. It underestimates `sales` for instances where the budget was split between the two media. This pronounced non-linear pattern suggests a *synergy* or *interaction* effect between the advertising media, whereby combining the media together results in a bigger boost to sales than using any single medium. In Section 3.3.2, we will discuss extending the linear model to accommodate such synergistic effects through the use of interaction terms.

interaction

Four: Predictions

Once we have fit the multiple regression model, it is straightforward to apply (3.21) in order to predict the response Y on the basis of a set of values for the predictors $X_1, X_2, \ldots, X_p$. However, there are three sorts of uncertainty associated with this prediction.

1. The coefficient estimates $\hat{\beta}_0, \hat{\beta}_1, \ldots, \hat{\beta}_p$ are estimates for $\beta_0, \beta_1, \ldots, \beta_p$. That is, the *least squares plane*

$$\hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 X_1 + \cdots + \hat{\beta}_p X_p$$

   is only an estimate for the *true population regression plane*

$$f(X) = \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p.$$

   The inaccuracy in the coefficient estimates is related to the *reducible error* from Chapter 2. We can compute a *confidence interval* in order to determine how close $\hat{Y}$ will be to $f(X)$.

2. Of course, in practice assuming a linear model for $f(X)$ is almost always an approximation of reality, so there is an additional source of potentially reducible error which we call *model bias*. So when we use a linear model, we are in fact estimating the best linear approximation to the true surface. However, here we will ignore this discrepancy, and operate as if the linear model were correct.

3. Even if we knew $f(X)$—that is, even if we knew the true values for $\beta_0, \beta_1, \ldots, \beta_p$—the response value cannot be predicted perfectly because of the random error ϵ in the model (3.20). In Chapter 2, we referred to this as the *irreducible error*. How much will Y vary from $\hat{Y}$? We use *prediction intervals* to answer this question. Prediction intervals are always wider than confidence intervals, because they incorporate both the error in the estimate for $f(X)$ (the reducible error) and the uncertainty as to how much an individual point will differ from the population regression plane (the irreducible error).

We use a *confidence interval* to quantify the uncertainty surrounding the *average* `sales` over a large number of cities. For example, given that \$100,000 is spent on `TV` advertising and \$20,000 is spent on `radio` advertising in each city, the 95 % confidence interval is [10,985, 11,528]. We interpret this to mean that 95 % of intervals of this form will contain the true value of $f(X)$.[9] On the other hand, a *prediction interval* can be used to quantify the

confidence interval

prediction interval

[9] In other words, if we collect a large number of data sets like the `Advertising` data set, and we construct a confidence interval for the average `sales` on the basis of each data set (given \$100,000 in `TV` and \$20,000 in `radio` advertising), then 95 % of these confidence intervals will contain the true value of average `sales`.

uncertainty surrounding sales for a *particular* city. Given that $100,000 is spent on TV advertising and $20,000 is spent on radio advertising in that city the 95 % prediction interval is [7,930, 14,580]. We interpret this to mean that 95 % of intervals of this form will contain the true value of Y for this city. Note that both intervals are centered at 11,256, but that the prediction interval is substantially wider than the confidence interval, reflecting the increased uncertainty about sales for a given city in comparison to the average sales over many locations.

3.3 Other Considerations in the Regression Model

3.3.1 Qualitative Predictors

In our discussion so far, we have assumed that all variables in our linear regression model are *quantitative*. But in practice, this is not necessarily the case; often some predictors are *qualitative*.

For example, the Credit data set displayed in Figure 3.6 records variables for a number of credit card holders. The response is balance (average credit card debt for each individual) and there are several quantitative predictors: age, cards (number of credit cards), education (years of education), income (in thousands of dollars), limit (credit limit), and rating (credit rating). Each panel of Figure 3.6 is a scatterplot for a pair of variables whose identities are given by the corresponding row and column labels. For example, the scatterplot directly to the right of the word "Balance" depicts balance versus age, while the plot directly to the right of "Age" corresponds to age versus cards. In addition to these quantitative variables, we also have four qualitative variables: own (house ownership), student (student status), status (marital status), and region (East, West or South).

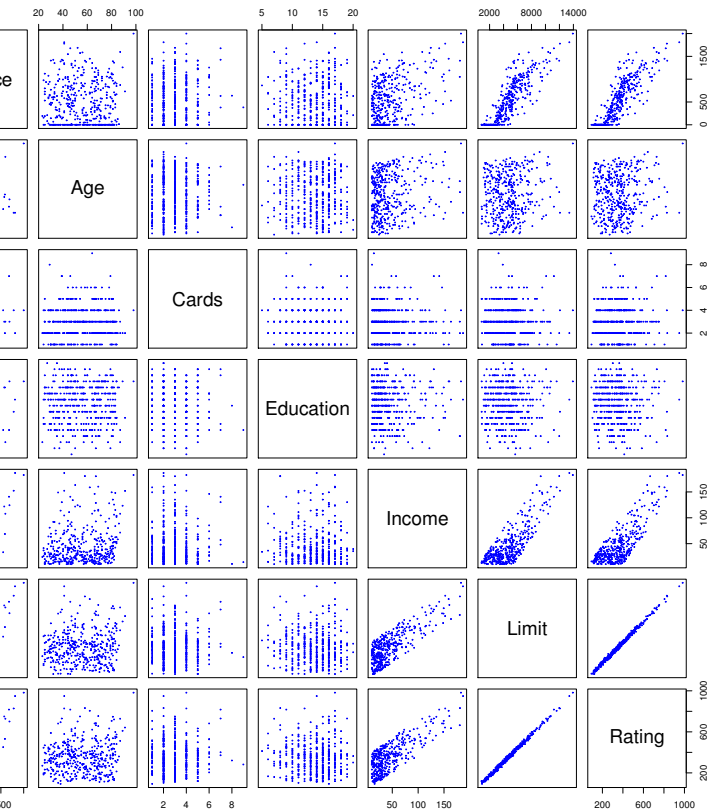
Predictors with Only Two Levels

Suppose that we wish to investigate differences in credit card balance between those who own a house and those who don't, ignoring the other variables for the moment. If a qualitative predictor (also known as a *factor*) only has two *levels*, or possible values, then incorporating it into a regression model is very simple. We simply create an indicator or *dummy variable* that takes on two possible numerical values.[10] For example, based on the own variable, we can create a new variable that takes the form

factor
level
dummy variable

$$x_i = \begin{cases} 1 & \text{if } i\text{th person owns a house} \\ 0 & \text{if } i\text{th person does not own a house,} \end{cases} \tag{3.26}$$

[10]In the machine learning community, the creation of dummy variables to handle qualitative predictors is known as "one-hot encoding".



3.6. *The* `Credit` *data set contains information about* `balance`*,* `age`*,* `cation`*,* `income`*,* `limit`*, and* `rating` *for a number of potential cus-*

is variable as a predictor in the regression equation. This results
lel

$$\beta_1 x_i + \epsilon_i = \begin{cases} \beta_0 + \beta_1 + \epsilon_i & \text{if } i\text{th person owns a house} \\ \beta_0 + \epsilon_i & \text{if } i\text{th person does not.} \end{cases} \quad (3.27)$$

n be interpreted as the average credit card balance among those t own, $\beta_0 + \beta_1$ as the average credit card balance among those vn their house, and β_1 as the average difference in credit card etween owners and non-owners.

7 displays the coefficient estimates and other information asso- n the model (3.27). The average credit card debt for non-owners ed to be \$509.80, whereas owners are estimated to carry \$19.73 nal debt for a total of \$509.80 + \$19.73 = \$529.53. However, we

	Coefficient	Std. error	t-statistic	p-value
Intercept	509.80	33.13	15.389	< 0.0001
own[Yes]	19.73	46.05	0.429	0.6690

TABLE 3.7. *Least squares coefficient estimates associated with the regression of* balance *onto* own *in the* Credit *data set. The linear model is given in (3.27). That is, ownership is encoded as a dummy variable, as in (3.26).*

notice that the p-value for the dummy variable is very high. This indicates that there is no statistical evidence of a difference in average credit card balance based on house ownership.

The decision to code owners as 1 and non-owners as 0 in (3.27) is arbitrary, and has no effect on the regression fit, but does alter the interpretation of the coefficients. If we had coded non-owners as 1 and owners as 0, then the estimates for β_0 and β_1 would have been 529.53 and -19.73, respectively, leading once again to a prediction of credit card debt of \$529.53 − \$19.73 = \$509.80 for non-owners and a prediction of \$529.53 for owners. Alternatively, instead of a 0/1 coding scheme, we could create a dummy variable

$$x_i = \begin{cases} 1 & \text{if } i\text{th person owns a house} \\ -1 & \text{if } i\text{th person does not own a house} \end{cases}$$

and use this variable in the regression equation. This results in the model

$$y_i = \beta_0 + \beta_1 x_i + \epsilon_i = \begin{cases} \beta_0 + \beta_1 + \epsilon_i & \text{if } i\text{th person owns a house} \\ \beta_0 - \beta_1 + \epsilon_i & \text{if } i\text{th person does not own a house.} \end{cases}$$

Now β_0 can be interpreted as the overall average credit card balance (ignoring the house ownership effect), and β_1 is the amount by which house owners and non-owners have credit card balances that are above and below the average, respectively.[11] In this example, the estimate for β_0 is \$519.665, halfway between the non-owner and owner averages of \$509.80 and \$529.53. The estimate for β_1 is \$9.865, which is half of \$19.73, the average difference between owners and non-owners. It is important to note that the final predictions for the credit balances of owners and non-owners will be identical regardless of the coding scheme used. The only difference is in the way that the coefficients are interpreted.

Qualitative Predictors with More than Two Levels

When a qualitative predictor has more than two levels, a single dummy variable cannot represent all possible values. In this situation, we can create

[11] Technically β_0 is half the sum of the average debt for house owners and the average debt for non-house owners. Hence, β_0 is exactly equal to the overall average only if the two groups have an equal number of members.

additional dummy variables. For example, for the region variable we create two dummy variables. The first could be

$$x_{i1} = \begin{cases} 1 & \text{if } i\text{th person is from the South} \\ 0 & \text{if } i\text{th person is not from the South,} \end{cases} \tag{3.28}$$

and the second could be

$$x_{i2} = \begin{cases} 1 & \text{if } i\text{th person is from the West} \\ 0 & \text{if } i\text{th person is not from the West.} \end{cases} \tag{3.29}$$

Then both of these variables can be used in the regression equation, in order to obtain the model

$$y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \epsilon_i = \begin{cases} \beta_0 + \beta_1 + \epsilon_i & \text{if } i\text{th person is from the South} \\ \beta_0 + \beta_2 + \epsilon_i & \text{if } i\text{th person is from the West} \\ \beta_0 + \epsilon_i & \text{if } i\text{th person is from the East.} \end{cases} \tag{3.30}$$

Now β_0 can be interpreted as the average credit card balance for individuals from the East, β_1 can be interpreted as the difference in the average balance between people from the South versus the East, and β_2 can be interpreted as the difference in the average balance between those from the West versus the East. There will always be one fewer dummy variable than the number of levels. The level with no dummy variable—East in this example—is known as the *baseline*.

baseline

From Table 3.8, we see that the estimated balance for the baseline, East, is \$531.00. It is estimated that those in the South will have \$18.69 less debt than those in the East, and that those in the West will have \$12.50 less debt than those in the East. However, the p-values associated with the coefficient estimates for the two dummy variables are very large, suggesting no statistical evidence of a real difference in average credit card balance between South and East or between West and East.[12] Once again, the level selected as the baseline category is arbitrary, and the final predictions for each group will be the same regardless of this choice. However, the coefficients and their p-values do depend on the choice of dummy variable coding. Rather than rely on the individual coefficients, we can use an F-test to test $H_0 : \beta_1 = \beta_2 = 0$; this does not depend on the coding. This F-test has a p-value of 0.96, indicating that we cannot reject the null hypothesis that there is no relationship between balance and region.

Using this dummy variable approach presents no difficulties when incorporating both quantitative and qualitative predictors. For example, to regress balance on both a quantitative variable such as income and a qualitative variable such as student, we must simply create a dummy variable

[12]There could still in theory be a difference between South and West, although the data here does not suggest any difference.

	Coefficient	Std. error	t-statistic	p-value
Intercept	531.00	46.32	11.464	< 0.0001
region[South]	−12.50	56.68	−0.221	0.8260
region[West]	−18.69	65.02	−0.287	0.7740

TABLE 3.8. *Least squares coefficient estimates associated with the regression of* balance *onto* region *in the* Credit *data set. The linear model is given in (3.30). That is, region is encoded via two dummy variables (3.28) and (3.29).*

for student and then fit a multiple regression model using income and the dummy variable as predictors for credit card balance.

There are many different ways of coding qualitative variables besides the dummy variable approach taken here. All of these approaches lead to equivalent model fits, but the coefficients are different and have different interpretations, and are designed to measure particular *contrasts*. This topic is beyond the scope of the book.

contrast

3.3.2 Extensions of the Linear Model

The standard linear regression model (3.19) provides interpretable results and works quite well on many real-world problems. However, it makes several highly restrictive assumptions that are often violated in practice. Two of the most important assumptions state that the relationship between the predictors and response are *additive* and *linear*. The additivity assumption means that the association between a predictor X_j and the response Y does not depend on the values of the other predictors. The linearity assumption states that the change in the response Y associated with a one-unit change in X_j is constant, regardless of the value of X_j. In later chapters of this book, we examine a number of sophisticated methods that relax these two assumptions. Here, we briefly examine some common classical approaches for extending the linear model.

additive
linear

Removing the Additive Assumption

In our previous analysis of the Advertising data, we concluded that both TV and radio seem to be associated with sales. The linear models that formed the basis for this conclusion assumed that the effect on sales of increasing one advertising medium is independent of the amount spent on the other media. For example, the linear model (3.20) states that the average increase in sales associated with a one-unit increase in TV is always β_1, regardless of the amount spent on radio.

However, this simple model may be incorrect. Suppose that spending money on radio advertising actually increases the effectiveness of TV advertising, so that the slope term for TV should increase as radio increases. In this situation, given a fixed budget of $100,000, spending half on radio and half on TV may increase sales more than allocating the entire amount

to either TV or to radio. In marketing, this is known as a *synergy* effect, and in statistics it is referred to as an *interaction* effect. Figure 3.5 suggests that such an effect may be present in the advertising data. Notice that when levels of either TV or radio are low, then the true sales are lower than predicted by the linear model. But when advertising is split between the two media, then the model tends to underestimate sales.

Consider the standard linear regression model with two variables,

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \epsilon.$$

According to this model, a one-unit increase in X_1 is associated with an average increase in Y of β_1 units. Notice that the presence of X_2 does not alter this statement—that is, regardless of the value of X_2, a one-unit increase in X_1 is associated with a β_1-unit increase in Y. One way of extending this model is to include a third predictor, called an *interaction term*, which is constructed by computing the product of X_1 and X_2. This results in the model

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_1 X_2 + \epsilon. \tag{3.31}$$

How does inclusion of this interaction term relax the additive assumption? Notice that (3.31) can be rewritten as

$$\begin{aligned} Y &= \beta_0 + (\beta_1 + \beta_3 X_2) X_1 + \beta_2 X_2 + \epsilon \\ &= \beta_0 + \tilde{\beta}_1 X_1 + \beta_2 X_2 + \epsilon \end{aligned} \tag{3.32}$$

where $\tilde{\beta}_1 = \beta_1 + \beta_3 X_2$. Since $\tilde{\beta}_1$ is now a function of X_2, the association between X_1 and Y is no longer constant: a change in the value of X_2 will change the association between X_1 and Y. A similar argument shows that a change in the value of X_1 changes the association between X_2 and Y.

For example, suppose that we are interested in studying the productivity of a factory. We wish to predict the number of units produced on the basis of the number of production lines and the total number of workers. It seems likely that the effect of increasing the number of production lines will depend on the number of workers, since if no workers are available to operate the lines, then increasing the number of lines will not increase production. This suggests that it would be appropriate to include an interaction term between lines and workers in a linear model to predict units. Suppose that when we fit the model, we obtain

$$\begin{aligned} \texttt{units} &\approx 1.2 + 3.4 \times \texttt{lines} + 0.22 \times \texttt{workers} + 1.4 \times (\texttt{lines} \times \texttt{workers}) \\ &= 1.2 + (3.4 + 1.4 \times \texttt{workers}) \times \texttt{lines} + 0.22 \times \texttt{workers}. \end{aligned}$$

In other words, adding an additional line will increase the number of units produced by $3.4 + 1.4 \times$ workers. Hence the more workers we have, the stronger will be the effect of lines.

	Coefficient	Std. error	t-statistic	p-value
Intercept	6.7502	0.248	27.23	< 0.0001
TV	0.0191	0.002	12.70	< 0.0001
radio	0.0289	0.009	3.24	0.0014
TV×radio	0.0011	0.000	20.73	< 0.0001

TABLE 3.9. *For the* Advertising *data, least squares coefficient estimates associated with the regression of* sales *onto* TV *and* radio*, with an interaction term, as in (3.33).*

We now return to the Advertising example. A linear model that uses radio, TV, and an interaction between the two to predict sales takes the form

$$\begin{aligned} \texttt{sales} &= \beta_0 + \beta_1 \times \texttt{TV} + \beta_2 \times \texttt{radio} + \beta_3 \times (\texttt{radio} \times \texttt{TV}) + \epsilon \\ &= \beta_0 + (\beta_1 + \beta_3 \times \texttt{radio}) \times \texttt{TV} + \beta_2 \times \texttt{radio} + \epsilon. \end{aligned} \tag{3.33}$$

We can interpret β_3 as the increase in the effectiveness of TV advertising associated with a one-unit increase in radio advertising (or vice-versa). The coefficients that result from fitting the model (3.33) are given in Table 3.9.

The results in Table 3.9 strongly suggest that the model that includes the interaction term is superior to the model that contains only *main effects*. The p-value for the interaction term, TV×radio, is extremely low, indicating that there is strong evidence for $H_a : \beta_3 \neq 0$. In other words, it is clear that the true relationship is not additive. The R^2 for the model (3.33) is 96.8 %, compared to only 89.7 % for the model that predicts sales using TV and radio without an interaction term. This means that $(96.8 - 89.7)/(100 - 89.7) = 69\,\%$ of the variability in sales that remains after fitting the additive model has been explained by the interaction term. The coefficient estimates in Table 3.9 suggest that an increase in TV advertising of \$1,000 is associated with increased sales of $(\hat{\beta}_1 + \hat{\beta}_3 \times \texttt{radio}) \times 1{,}000 = 19 + 1.1 \times \texttt{radio}$ units. And an increase in radio advertising of \$1,000 will be associated with an increase in sales of $(\hat{\beta}_2 + \hat{\beta}_3 \times \texttt{TV}) \times 1{,}000 = 29 + 1.1 \times \texttt{TV}$ units.

main effect

In this example, the p-values associated with TV, radio, and the interaction term all are statistically significant (Table 3.9), and so it is obvious that all three variables should be included in the model. However, it is sometimes the case that an interaction term has a very small p-value, but the associated main effects (in this case, TV and radio) do not. The *hierarchical principle* states that *if we include an interaction in a model, we should also include the main effects, even if the p-values associated with their coefficients are not significant.* In other words, if the interaction between X_1 and X_2 seems important, then we should include both X_1 and X_2 in the model even if their coefficient estimates have large p-values. The rationale for this principle is that if $X_1 \times X_2$ is related to the response, then whether or not the coefficients of X_1 or X_2 are exactly zero is of lit-

hierarchical principle

tle interest. Also $X_1 \times X_2$ is typically correlated with X_1 and X_2, and so leaving them out tends to alter the meaning of the interaction.

In the previous example, we considered an interaction between TV and radio, both of which are quantitative variables. However, the concept of interactions applies just as well to qualitative variables, or to a combination of quantitative and qualitative variables. In fact, an interaction between a qualitative variable and a quantitative variable has a particularly nice interpretation. Consider the Credit data set from Section 3.3.1, and suppose that we wish to predict balance using the income (quantitative) and student (qualitative) variables. In the absence of an interaction term, the model takes the form

$$\begin{aligned} \texttt{balance}_i &\approx \beta_0 + \beta_1 \times \texttt{income}_i + \begin{cases} \beta_2 & \text{if } i\text{th person is a student} \\ 0 & \text{if } i\text{th person is not a student} \end{cases} \\ &= \beta_1 \times \texttt{income}_i + \begin{cases} \beta_0 + \beta_2 & \text{if } i\text{th person is a student} \\ \beta_0 & \text{if } i\text{th person is not a student.} \end{cases} \end{aligned} \tag{3.34}$$

Notice that this amounts to fitting two parallel lines to the data, one for students and one for non-students. The lines for students and non-students have different intercepts, $\beta_0 + \beta_2$ versus β_0, but the same slope, β_1. This is illustrated in the left-hand panel of Figure 3.7. The fact that the lines are parallel means that the average effect on balance of a one-unit increase in income does not depend on whether or not the individual is a student. This represents a potentially serious limitation of the model, since in fact a change in income may have a very different effect on the credit card balance of a student versus a non-student.

This limitation can be addressed by adding an interaction variable, created by multiplying income with the dummy variable for student. Our model now becomes

$$\begin{aligned} \texttt{balance}_i &\approx \beta_0 + \beta_1 \times \texttt{income}_i + \begin{cases} \beta_2 + \beta_3 \times \texttt{income}_i & \text{if student} \\ 0 & \text{if not student} \end{cases} \\ &= \begin{cases} (\beta_0 + \beta_2) + (\beta_1 + \beta_3) \times \texttt{income}_i & \text{if student} \\ \beta_0 + \beta_1 \times \texttt{income}_i & \text{if not student.} \end{cases} \end{aligned} \tag{3.35}$$

Once again, we have two different regression lines for the students and the non-students. But now those regression lines have different intercepts, $\beta_0+\beta_2$ versus β_0, as well as different slopes, $\beta_1+\beta_3$ versus β_1. This allows for the possibility that changes in income may affect the credit card balances of students and non-students differently. The right-hand panel of Figure 3.7 shows the estimated relationships between income and balance for students

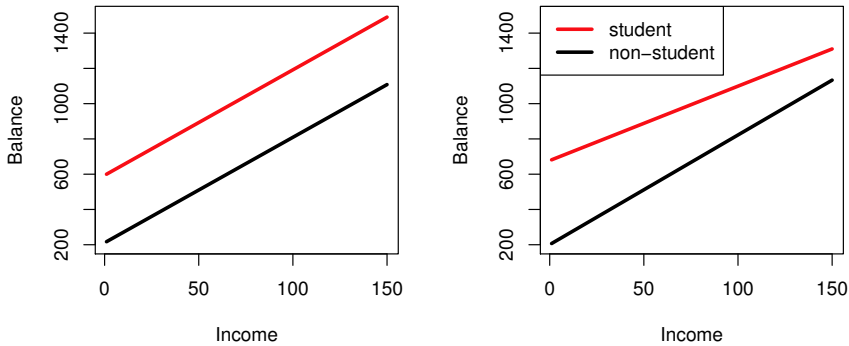


FIGURE 3.7. *For the* `Credit` *data, the least squares lines are shown for prediction of* `balance` *from* `income` *for students and non-students.* Left: *The model (3.34) was fit. There is no interaction between* `income` *and* `student`*.* Right: *The model (3.35) was fit. There is an interaction term between* `income` *and* `student`*.*

and non-students in the model (3.35). We note that the slope for students is lower than the slope for non-students. This suggests that increases in income are associated with smaller increases in credit card balance among students as compared to non-students.

Non-linear Relationships

As discussed previously, the linear regression model (3.19) assumes a linear relationship between the response and predictors. But in some cases, the true relationship between the response and the predictors may be non-linear. Here we present a very simple way to directly extend the linear model to accommodate non-linear relationships, using *polynomial regression*. In later chapters, we will present more complex approaches for performing non-linear fits in more general settings.

polynomial regression

Consider Figure 3.8, in which the `mpg` (gas mileage in miles per gallon) versus `horsepower` is shown for a number of cars in the `Auto` data set. The orange line represents the linear regression fit. There is a pronounced relationship between `mpg` and `horsepower`, but it seems clear that this relationship is in fact non-linear: the data suggest a curved relationship. A simple approach for incorporating non-linear associations in a linear model is to include transformed versions of the predictors. For example, the points in Figure 3.8 seem to have a *quadratic* shape, suggesting that a model of the form

quadratic

$$\texttt{mpg} = \beta_0 + \beta_1 \times \texttt{horsepower} + \beta_2 \times \texttt{horsepower}^2 + \epsilon \tag{3.36}$$

may provide a better fit. Equation 3.36 involves predicting `mpg` using a non-linear function of `horsepower`. *But it is still a linear model!* That is, (3.36) is simply a multiple linear regression model with $X_1 =$ `horsepower`

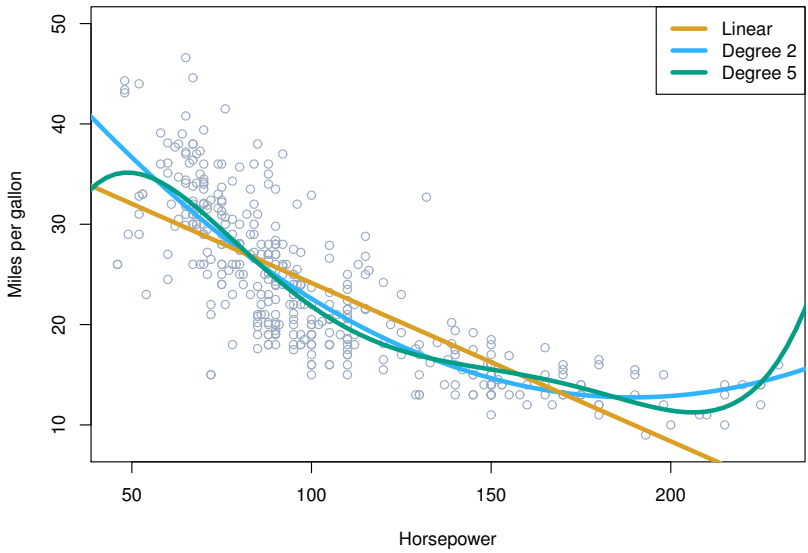


FIGURE 3.8. *The* `Auto` *data set. For a number of cars,* `mpg` *and* `horsepower` *are shown. The linear regression fit is shown in orange. The linear regression fit for a model that includes* $\texttt{horsepower}^2$ *is shown as a blue curve. The linear regression fit for a model that includes all polynomials of* `horsepower` *up to fifth-degree is shown in green.*

	Coefficient	Std. error	t-statistic	p-value
`Intercept`	56.9001	1.8004	31.6	< 0.0001
`horsepower`	−0.4662	0.0311	−15.0	< 0.0001
$\texttt{horsepower}^2$	0.0012	0.0001	10.1	< 0.0001

TABLE 3.10. *For the* `Auto` *data set, least squares coefficient estimates associated with the regression of* `mpg` *onto* `horsepower` *and* $\texttt{horsepower}^2$.

and $X_2 = \texttt{horsepower}^2$. So we can use standard linear regression software to estimate β_0, β_1, and β_2 in order to produce a non-linear fit. The blue curve in Figure 3.8 shows the resulting quadratic fit to the data. The quadratic fit appears to be substantially better than the fit obtained when just the linear term is included. The R^2 of the quadratic fit is 0.688, compared to 0.606 for the linear fit, and the p-value in Table 3.10 for the quadratic term is highly significant.

If including $\texttt{horsepower}^2$ led to such a big improvement in the model, why not include $\texttt{horsepower}^3$, $\texttt{horsepower}^4$, or even $\texttt{horsepower}^5$? The green curve in Figure 3.8 displays the fit that results from including all polynomials up to fifth degree in the model (3.36). The resulting fit seems unnecessarily wiggly—that is, it is unclear that including the additional terms really has led to a better fit to the data.

The approach that we have just described for extending the linear model to accommodate non-linear relationships is known as *polynomial regression*, since we have included polynomial functions of the predictors in the regression model. We further explore this approach and other non-linear extensions of the linear model in Chapter 7.

3.3.3 Potential Problems

When we fit a linear regression model to a particular data set, many problems may occur. Most common among these are the following:

1. *Non-linearity of the response-predictor relationships.*
2. *Correlation of error terms.*
3. *Non-constant variance of error terms.*
4. *Outliers.*
5. *High-leverage points.*
6. *Collinearity.*

In practice, identifying and overcoming these problems is as much an art as a science. Many pages in countless books have been written on this topic. Since the linear regression model is not our primary focus here, we will provide only a brief summary of some key points.

1. Non-linearity of the Data

The linear regression model assumes that there is a straight-line relationship between the predictors and the response. If the true relationship is far from linear, then virtually all of the conclusions that we draw from the fit are suspect. In addition, the prediction accuracy of the model can be significantly reduced.

Residual plots are a useful graphical tool for identifying non-linearity. Given a simple linear regression model, we can plot the residuals, $e_i = y_i - \hat{y}_i$, versus the predictor x_i. In the case of a multiple regression model, since there are multiple predictors, we instead plot the residuals versus the predicted (or *fitted*) values $\hat{y}_i$. Ideally, the residual plot will show no discernible pattern. The presence of a pattern may indicate a problem with some aspect of the linear model.

residual plot

fitted

The left panel of Figure 3.9 displays a residual plot from the linear regression of `mpg` onto `horsepower` on the `Auto` data set that was illustrated in Figure 3.8. The red line is a smooth fit to the residuals, which is displayed in order to make it easier to identify any trends. The residuals exhibit a clear U-shape, which provides a strong indication of non-linearity in the data. In contrast, the right-hand panel of Figure 3.9 displays the residual plot

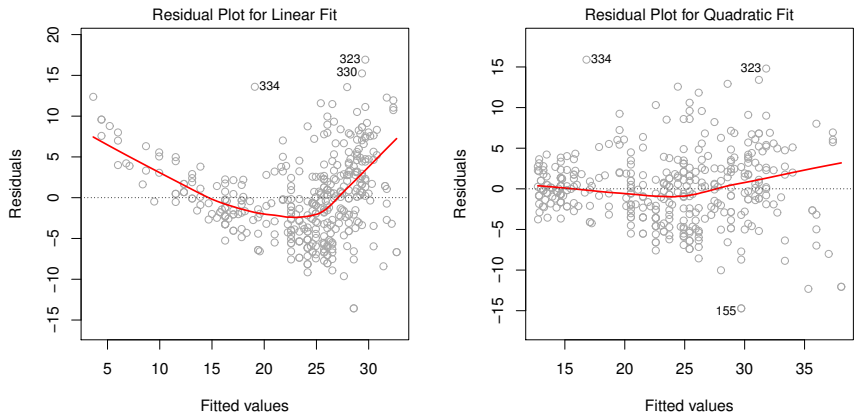


FIGURE 3.9. *Plots of residuals versus predicted (or fitted) values for the* `Auto` *data set. In each plot, the red line is a smooth fit to the residuals, intended to make it easier to identify a trend.* Left: *A linear regression of* `mpg` *on* `horsepower`*. A strong pattern in the residuals indicates non-linearity in the data.* Right: *A linear regression of* `mpg` *on* `horsepower` *and* $\texttt{horsepower}^2$*. There is little pattern in the residuals.*

that results from the model (3.36), which contains a quadratic term. There appears to be little pattern in the residuals, suggesting that the quadratic term improves the fit to the data.

If the residual plot indicates that there are non-linear associations in the data, then a simple approach is to use non-linear transformations of the predictors, such as $\log X$, $\sqrt{X}$, and X^2, in the regression model. In the later chapters of this book, we will discuss other more advanced non-linear approaches for addressing this issue.

2. Correlation of Error Terms

An important assumption of the linear regression model is that the error terms, $\epsilon_1, \epsilon_2, \ldots, \epsilon_n$, are uncorrelated. What does this mean? For instance, if the errors are uncorrelated, then the fact that ϵ_i is positive provides little or no information about the sign of ϵ_{i+1}. The standard errors that are computed for the estimated regression coefficients or the fitted values are based on the assumption of uncorrelated error terms. If in fact there is correlation among the error terms, then the estimated standard errors will tend to underestimate the true standard errors. As a result, confidence and prediction intervals will be narrower than they should be. For example, a 95 % confidence interval may in reality have a much lower probability than 0.95 of containing the true value of the parameter. In addition, p-values associated with the model will be lower than they should be; this could cause us to erroneously conclude that a parameter is statistically

significant. In short, if the error terms are correlated, we may have an unwarranted sense of confidence in our model.

As an extreme example, suppose we accidentally doubled our data, leading to observations and error terms identical in pairs. If we ignored this, our standard error calculations would be as if we had a sample of size $2n$, when in fact we have only n samples. Our estimated parameters would be the same for the $2n$ samples as for the n samples, but the confidence intervals would be narrower by a factor of $\sqrt{2}$!

Why might correlations among the error terms occur? Such correlations frequently occur in the context of *time series* data, which consists of observations for which measurements are obtained at discrete points in time. In many cases, observations that are obtained at adjacent time points will have positively correlated errors. In order to determine if this is the case for a given data set, we can plot the residuals from our model as a function of time. If the errors are uncorrelated, then there should be no discernible pattern. On the other hand, if the error terms are positively correlated, then we may see *tracking* in the residuals—that is, adjacent residuals may have similar values. Figure 3.10 provides an illustration. In the top panel, we see the residuals from a linear regression fit to data generated with uncorrelated errors. There is no evidence of a time-related trend in the residuals. In contrast, the residuals in the bottom panel are from a data set in which adjacent errors had a correlation of 0.9. Now there is a clear pattern in the residuals—adjacent residuals tend to take on similar values. Finally, the center panel illustrates a more moderate case in which the residuals had a correlation of 0.5. There is still evidence of tracking, but the pattern is less clear.

time series

tracking

Many methods have been developed to properly take account of correlations in the error terms in time series data. Correlation among the error terms can also occur outside of time series data. For instance, consider a study in which individuals' heights are predicted from their weights. The assumption of uncorrelated errors could be violated if some of the individuals in the study are members of the same family, eat the same diet, or have been exposed to the same environmental factors. In general, the assumption of uncorrelated errors is extremely important for linear regression as well as for other statistical methods, and good experimental design is crucial in order to mitigate the risk of such correlations.

3. Non-constant Variance of Error Terms

Another important assumption of the linear regression model is that the error terms have a constant variance, $\text{Var}(\epsilon_i) = \sigma^2$. The standard errors, confidence intervals, and hypothesis tests associated with the linear model rely upon this assumption.

Unfortunately, it is often the case that the variances of the error terms are non-constant. For instance, the variances of the error terms may increase

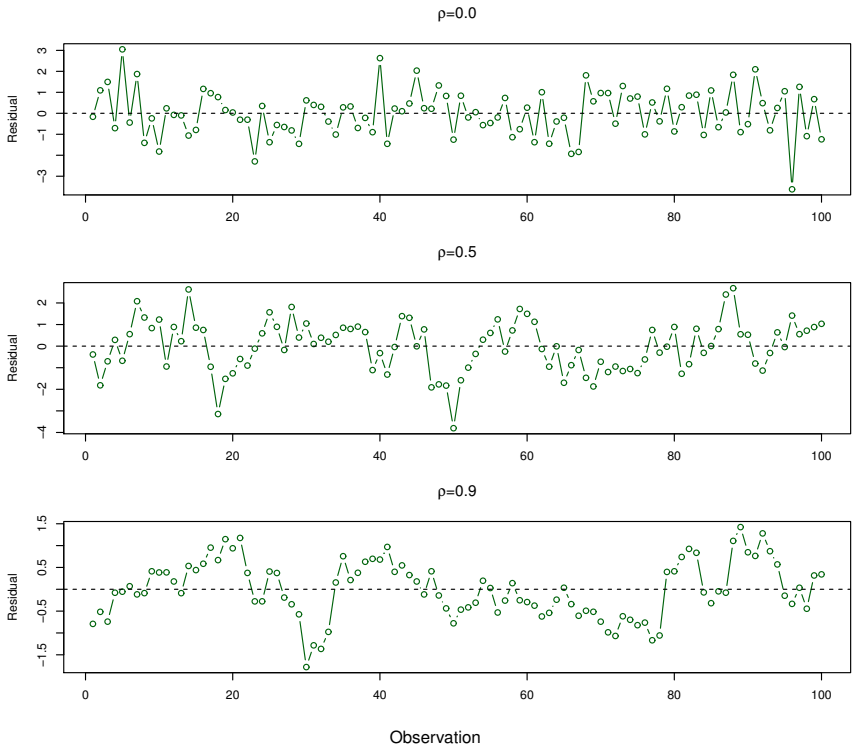


FIGURE 3.10. *Plots of residuals from simulated time series data sets generated with differing levels of correlation ρ between error terms for adjacent time points.*

with the value of the response. One can identify non-constant variances in the errors, or *heteroscedasticity*, from the presence of a *funnel shape* in the residual plot. An example is shown in the left-hand panel of Figure 3.11, in which the magnitude of the residuals tends to increase with the fitted values. When faced with this problem, one possible solution is to transform the response Y using a concave function such as $\log Y$ or $\sqrt{Y}$. Such a transformation results in a greater amount of shrinkage of the larger responses, leading to a reduction in heteroscedasticity. The right-hand panel of Figure 3.11 displays the residual plot after transforming the response using $\log Y$. The residuals now appear to have constant variance, though there is some evidence of a slight non-linear relationship in the data.

hetero-
scedasticity

Sometimes we have a good idea of the variance of each response. For example, the ith response could be an average of n_i raw observations. If each of these raw observations is uncorrelated with variance σ^2, then their average has variance $\sigma_i^2 = \sigma^2/n_i$. In this case a simple remedy is to fit our model by *weighted least squares*, with weights proportional to the inverse

weighted
least squares

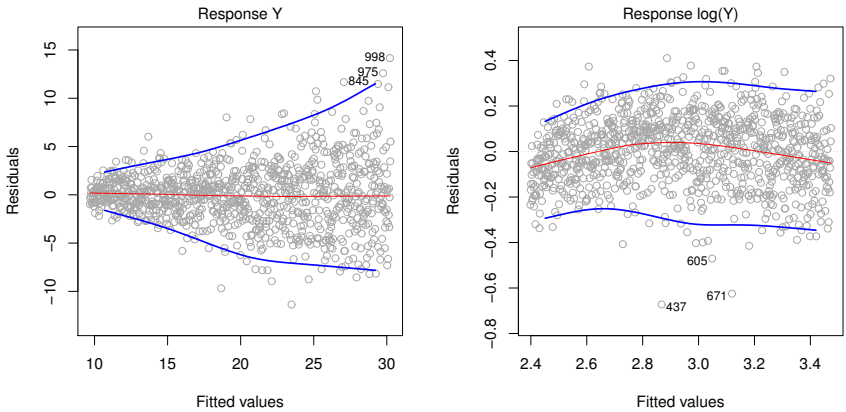


FIGURE 3.11. *Residual plots. In each plot, the red line is a smooth fit to the residuals, intended to make it easier to identify a trend. The blue lines track the outer quantiles of the residuals, and emphasize patterns.* Left: *The funnel shape indicates heteroscedasticity.* Right: *The response has been log transformed, and there is now no evidence of heteroscedasticity.*

variances—i.e. $w_i = n_i$ in this case. Most linear regression software allows for observation weights.

4. Outliers

An *outlier* is a point for which y_i is far from the value predicted by the model. Outliers can arise for a variety of reasons, such as incorrect recording of an observation during data collection. outlier

The red point (observation 20) in the left-hand panel of Figure 3.12 illustrates a typical outlier. The red solid line is the least squares regression fit, while the blue dashed line is the least squares fit after removal of the outlier. In this case, removing the outlier has little effect on the least squares line: it leads to almost no change in the slope, and a miniscule reduction in the intercept. It is typical for an outlier that does not have an unusual predictor value to have little effect on the least squares fit. However, even if an outlier does not have much effect on the least squares fit, it can cause other problems. For instance, in this example, the RSE is 1.09 when the outlier is included in the regression, but it is only 0.77 when the outlier is removed. Since the RSE is used to compute all confidence intervals and p-values, such a dramatic increase caused by a single data point can have implications for the interpretation of the fit. Similarly, inclusion of the outlier causes the R^2 to decline from 0.892 to 0.805.

Residual plots can be used to identify outliers. In this example, the outlier is clearly visible in the residual plot illustrated in the center panel of Figure 3.12. But in practice, it can be difficult to decide how large a resid-

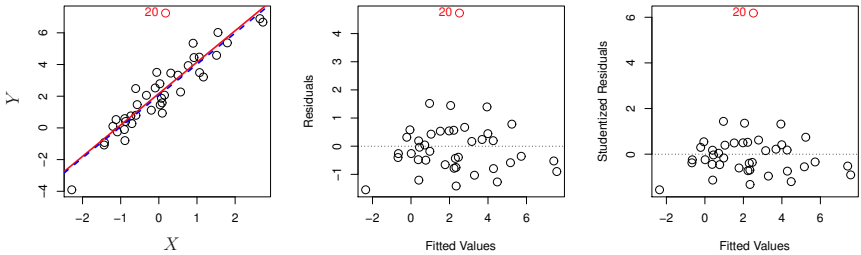


FIGURE 3.12. Left: *The least squares regression line is shown in red, and the regression line after removing the outlier is shown in blue.* Center: *The residual plot clearly identifies the outlier.* Right: *The outlier has a studentized residual of* 6*; typically we expect values between* -3 *and* 3*.*

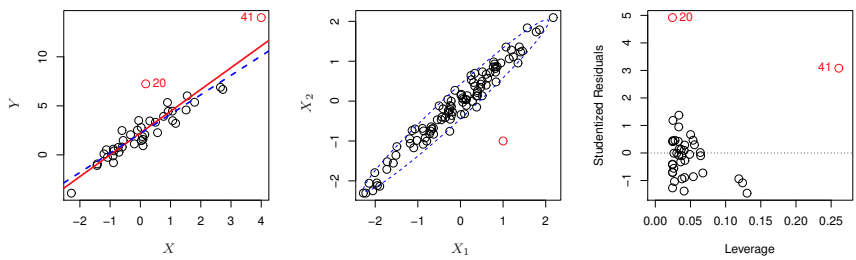


FIGURE 3.13. Left: *Observation 41 is a high leverage point, while 20 is not. The red line is the fit to all the data, and the blue line is the fit with observation 41 removed.* Center: *The red observation is not unusual in terms of its* X_1 *value or its* X_2 *value, but still falls outside the bulk of the data, and hence has high leverage.* Right: *Observation* 41 *has a high leverage and a high residual.*

ual needs to be before we consider the point to be an outlier. To address this problem, instead of plotting the residuals, we can plot the *studentized residuals*, computed by dividing each residual e_i by its estimated standard error. Observations whose studentized residuals are greater than 3 in absolute value are possible outliers. In the right-hand panel of Figure 3.12, the outlier's studentized residual exceeds 6, while all other observations have studentized residuals between -2 and 2.

studentized residual

If we believe that an outlier has occurred due to an error in data collection or recording, then one solution is to simply remove the observation. However, care should be taken, since an outlier may instead indicate a deficiency with the model, such as a missing predictor.

5. High Leverage Points

We just saw that outliers are observations for which the response y_i is unusual given the predictor x_i. In contrast, observations with *high leverage*

high leverage

have an unusual value for x_i. For example, observation 41 in the left-hand panel of Figure 3.13 has high leverage, in that the predictor value for this observation is large relative to the other observations. (Note that the data displayed in Figure 3.13 are the same as the data displayed in Figure 3.12, but with the addition of a single high leverage observation.) The red solid line is the least squares fit to the data, while the blue dashed line is the fit produced when observation 41 is removed. Comparing the left-hand panels of Figures 3.12 and 3.13, we observe that removing the high leverage observation has a much more substantial impact on the least squares line than removing the outlier. In fact, high leverage observations tend to have a sizable impact on the estimated regression line. It is cause for concern if the least squares line is heavily affected by just a couple of observations, because any problems with these points may invalidate the entire fit. For this reason, it is important to identify high leverage observations.

In a simple linear regression, high leverage observations are fairly easy to identify, since we can simply look for observations for which the predictor value is outside of the normal range of the observations. But in a multiple linear regression with many predictors, it is possible to have an observation that is well within the range of each individual predictor's values, but that is unusual in terms of the full set of predictors. An example is shown in the center panel of Figure 3.13, for a data set with two predictors, X_1 and X_2. Most of the observations' predictor values fall within the blue dashed ellipse, but the red observation is well outside of this range. But neither its value for X_1 nor its value for X_2 is unusual. So if we examine just X_1 or just X_2, we will fail to notice this high leverage point. This problem is more pronounced in multiple regression settings with more than two predictors, because then there is no simple way to plot all dimensions of the data simultaneously.

In order to quantify an observation's leverage, we compute the *leverage statistic*. A large value of this statistic indicates an observation with high leverage. For a simple linear regression,

leverage statistic

$$h_i = \frac{1}{n} + \frac{(x_i - \bar{x})^2}{\sum_{i'=1}^{n}(x_{i'} - \bar{x})^2}. \tag{3.37}$$

It is clear from this equation that h_i increases with the distance of x_i from $\bar{x}$. There is a simple extension of h_i to the case of multiple predictors, though we do not provide the formula here. The leverage statistic h_i is always between $1/n$ and 1, and the average leverage for all the observations is always equal to $(p+1)/n$. So if a given observation has a leverage statistic that greatly exceeds $(p+1)/n$, then we may suspect that the corresponding point has high leverage.

The right-hand panel of Figure 3.13 provides a plot of the studentized residuals versus h_i for the data in the left-hand panel of Figure 3.13. Observation 41 stands out as having a very high leverage statistic as well as a high studentized residual. In other words, it is an outlier as well as a high

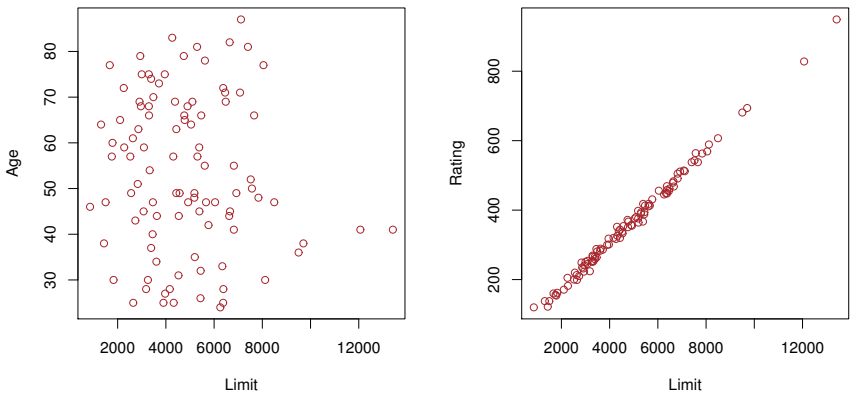


FIGURE 3.14. *Scatterplots of the observations from the* `Credit` *data set.* Left: *A plot of* `age` *versus* `limit`*. These two variables are not collinear.* Right: *A plot of* `rating` *versus* `limit`*. There is high collinearity.*

leverage observation. This is a particularly dangerous combination! This plot also reveals the reason that observation 20 had relatively little effect on the least squares fit in Figure 3.12: it has low leverage.

6. Collinearity

Collinearity refers to the situation in which two or more predictor variables are closely related to one another. The concept of collinearity is illustrated in Figure 3.14 using the `Credit` data set. In the left-hand panel of Figure 3.14, the two predictors `limit` and `age` appear to have no obvious relationship. In contrast, in the right-hand panel of Figure 3.14, the predictors `limit` and `rating` are very highly correlated with each other, and we say that they are *collinear*. The presence of collinearity can pose problems in the regression context, since it can be difficult to separate out the individual effects of collinear variables on the response. In other words, since `limit` and `rating` tend to increase or decrease together, it can be difficult to determine how each one separately is associated with the response, `balance`.

collinearity

Figure 3.15 illustrates some of the difficulties that can result from collinearity. The left-hand panel of Figure 3.15 is a contour plot of the RSS (3.22) associated with different possible coefficient estimates for the regression of `balance` on `limit` and `age`. Each ellipse represents a set of coefficients that correspond to the same RSS, with ellipses nearest to the center taking on the lowest values of RSS. The black dots and associated dashed lines represent the coefficient estimates that result in the smallest possible RSS—in other words, these are the least squares estimates. The axes for `limit` and `age` have been scaled so that the plot includes possible coefficient estimates that are up to four standard errors on either side of the least squares estimates. Thus the plot includes all plausible values for the

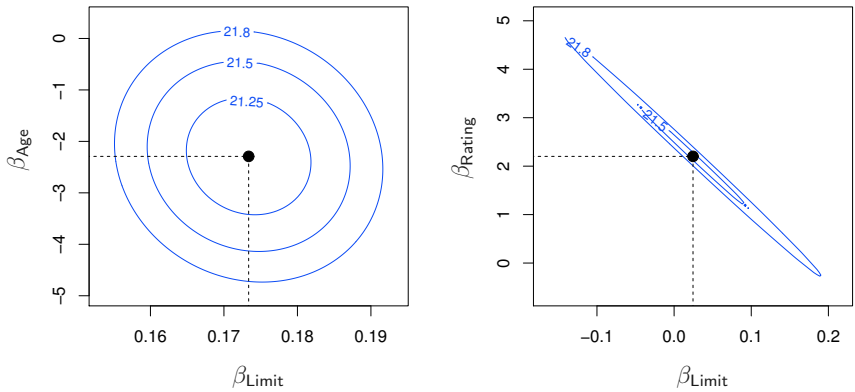


FIGURE 3.15. *Contour plots for the RSS values as a function of the parameters β for various regressions involving the* `Credit` *data set. In each plot, the black dots represent the coefficient values corresponding to the minimum RSS.* Left: *A contour plot of RSS for the regression of* `balance` *onto* `age` *and* `limit`*. The minimum value is well defined.* Right: *A contour plot of RSS for the regression of* `balance` *onto* `rating` *and* `limit`*. Because of the collinearity, there are many pairs* $(\beta_{\text{Limit}}, \beta_{\text{Rating}})$ *with a similar value for RSS.*

coefficients. For example, we see that the true `limit` coefficient is almost certainly somewhere between 0.15 and 0.20.

In contrast, the right-hand panel of Figure 3.15 displays contour plots of the RSS associated with possible coefficient estimates for the regression of `balance` onto `limit` and `rating`, which we know to be highly collinear. Now the contours run along a narrow valley; there is a broad range of values for the coefficient estimates that result in equal values for RSS. Hence a small change in the data could cause the pair of coefficient values that yield the smallest RSS—that is, the least squares estimates—to move anywhere along this valley. This results in a great deal of uncertainty in the coefficient estimates. Notice that the scale for the `limit` coefficient now runs from roughly −0.2 to 0.2; this is an eight-fold increase over the plausible range of the `limit` coefficient in the regression with `age`. Interestingly, even though the `limit` and `rating` coefficients now have much more individual uncertainty, they will almost certainly lie somewhere in this contour valley. For example, we would not expect the true value of the `limit` and `rating` coefficients to be −0.1 and 1 respectively, even though such a value is plausible for each coefficient individually.

Since collinearity reduces the accuracy of the estimates of the regression coefficients, it causes the standard error for $\hat{\beta}_j$ to grow. Recall that the t-statistic for each predictor is calculated by dividing $\hat{\beta}_j$ by its standard error. Consequently, collinearity results in a decline in the t-statistic. As a result, in the presence of collinearity, we may fail to reject $H_0 : \beta_j = 0$. This

		Coefficient	Std. error	t-statistic	p-value
Model 1	Intercept	−173.411	43.828	−3.957	< 0.0001
	age	−2.292	0.672	−3.407	0.0007
	limit	0.173	0.005	34.496	< 0.0001
Model 2	Intercept	−377.537	45.254	−8.343	< 0.0001
	rating	2.202	0.952	2.312	0.0213
	limit	0.025	0.064	0.384	0.7012

TABLE 3.11. *The results for two multiple regression models involving the* Credit *data set are shown. Model 1 is a regression of* balance *on* age *and* limit*, and Model 2 a regression of* balance *on* rating *and* limit*. The standard error of* $\hat{\beta}_{\text{limit}}$ *increases 12-fold in the second regression, due to collinearity.*

means that the *power* of the hypothesis test—the probability of correctly detecting a *non-zero* coefficient—is reduced by collinearity.

power

Table 3.11 compares the coefficient estimates obtained from two separate multiple regression models. The first is a regression of balance on age and limit, and the second is a regression of balance on rating and limit. In the first regression, both age and limit are highly significant with very small p-values. In the second, the collinearity between limit and rating has caused the standard error for the limit coefficient estimate to increase by a factor of 12 and the p-value to increase to 0.701. In other words, the importance of the limit variable has been masked due to the presence of collinearity. To avoid such a situation, it is desirable to identify and address potential collinearity problems while fitting the model.

A simple way to detect collinearity is to look at the correlation matrix of the predictors. An element of this matrix that is large in absolute value indicates a pair of highly correlated variables, and therefore a collinearity problem in the data. Unfortunately, not all collinearity problems can be detected by inspection of the correlation matrix: it is possible for collinearity to exist between three or more variables even if no pair of variables has a particularly high correlation. We call this situation *multicollinearity*. Instead of inspecting the correlation matrix, a better way to assess multicollinearity is to compute the *variance inflation factor* (VIF). The VIF is the ratio of the variance of $\hat{\beta}_j$ when fitting the full model divided by the variance of $\hat{\beta}_j$ if fit on its own. The smallest possible value for VIF is 1, which indicates the complete absence of collinearity. Typically in practice there is a small amount of collinearity among the predictors. As a rule of thumb, a VIF value that exceeds 5 or 10 indicates a problematic amount of collinearity. The VIF for each variable can be computed using the formula

multicollinearity

variance inflation factor

$$\text{VIF}(\hat{\beta}_j) = \frac{1}{1 - R^2_{X_j|X_{-j}}},$$

where $R^2_{X_j|X_{-j}}$ is the R^2 from a regression of X_j onto all of the other predictors. If $R^2_{X_j|X_{-j}}$ is close to one, then collinearity is present, and so the VIF will be large.

In the `Credit` data, a regression of `balance` on `age`, `rating`, and `limit` indicates that the predictors have VIF values of 1.01, 160.67, and 160.59. As we suspected, there is considerable collinearity in the data!

When faced with the problem of collinearity, there are two simple solutions. The first is to drop one of the problematic variables from the regression. This can usually be done without much compromise to the regression fit, since the presence of collinearity implies that the information that this variable provides about the response is redundant in the presence of the other variables. For instance, if we regress `balance` onto `age` and `limit`, without the `rating` predictor, then the resulting VIF values are close to the minimum possible value of 1, and the R^2 drops from 0.754 to 0.75. So dropping `rating` from the set of predictors has effectively solved the collinearity problem without compromising the fit. The second solution is to combine the collinear variables together into a single predictor. For instance, we might take the average of standardized versions of `limit` and `rating` in order to create a new variable that measures *credit worthiness*.

3.4 The Marketing Plan

We now briefly return to the seven questions about the `Advertising` data that we set out to answer at the beginning of this chapter.

1. *Is there a relationship between sales and advertising budget?*
   This question can be answered by fitting a multiple regression model of `sales` onto `TV`, `radio`, and `newspaper`, as in (3.20), and testing the hypothesis $H_0 : \beta_{\texttt{TV}} = \beta_{\texttt{radio}} = \beta_{\texttt{newspaper}} = 0$. In Section 3.2.2, we showed that the F-statistic can be used to determine whether or not we should reject this null hypothesis. In this case the p-value corresponding to the F-statistic in Table 3.6 is very low, indicating clear evidence of a relationship between advertising and sales.

2. *How strong is the relationship?*
   We discussed two measures of model accuracy in Section 3.1.3. First, the RSE estimates the standard deviation of the response from the population regression line. For the `Advertising` data, the RSE is 1.69 units while the mean value for the response is 14.022, indicating a percentage error of roughly 12 %. Second, the R^2 statistic records the percentage of variability in the response that is explained by the predictors. The predictors explain almost 90 % of the variance in `sales`. The RSE and R^2 statistics are displayed in Table 3.6.

3. *Which media are associated with sales?*
To answer this question, we can examine the p-values associated with each predictor's t-statistic (Section 3.1.2). In the multiple linear regression displayed in Table 3.4, the p-values for `TV` and `radio` are low, but the p-value for `newspaper` is not. This suggests that only `TV` and `radio` are related to `sales`. In Chapter 6 we explore this question in greater detail.

4. *How large is the association between each medium and sales?*
We saw in Section 3.1.2 that the standard error of $\hat{\beta}_j$ can be used to construct confidence intervals for β_j. For the `Advertising` data, we can use the results in Table 3.4 to compute the 95 % confidence intervals for the coefficients in a multiple regression model using all three media budgets as predictors. The confidence intervals are as follows: $(0.043, 0.049)$ for `TV`, $(0.172, 0.206)$ for `radio`, and $(-0.013, 0.011)$ for `newspaper`. The confidence intervals for `TV` and `radio` are narrow and far from zero, providing evidence that these media are related to `sales`. But the interval for `newspaper` includes zero, indicating that the variable is not statistically significant given the values of `TV` and `radio`.

   We saw in Section 3.3.3 that collinearity can result in very wide standard errors. Could collinearity be the reason that the confidence interval associated with `newspaper` is so wide? The VIF scores are 1.005, 1.145, and 1.145 for `TV`, `radio`, and `newspaper`, suggesting no evidence of collinearity.

   In order to assess the association of each medium individually on sales, we can perform three separate simple linear regressions. Results are shown in Tables 3.1 and 3.3. There is evidence of an extremely strong association between `TV` and `sales` and between `radio` and `sales`. There is evidence of a mild association between `newspaper` and `sales`, when the values of `TV` and `radio` are ignored.

5. *How accurately can we predict future sales?*
The response can be predicted using (3.21). The accuracy associated with this estimate depends on whether we wish to predict an individual response, $Y = f(X) + \epsilon$, or the average response, $f(X)$ (Section 3.2.2). If the former, we use a prediction interval, and if the latter, we use a confidence interval. Prediction intervals will always be wider than confidence intervals because they account for the uncertainty associated with ϵ, the irreducible error.

6. *Is the relationship linear?*
In Section 3.3.3, we saw that residual plots can be used in order to identify non-linearity. If the relationships are linear, then the residual plots should display no pattern. In the case of the `Advertising` data,

we observe a non-linear effect in Figure 3.5, though this effect could also be observed in a residual plot. In Section 3.3.2, we discussed the inclusion of transformations of the predictors in the linear regression model in order to accommodate non-linear relationships.

7. *Is there synergy among the advertising media?*
The standard linear regression model assumes an additive relationship between the predictors and the response. An additive model is easy to interpret because the association between each predictor and the response is unrelated to the values of the other predictors. However, the additive assumption may be unrealistic for certain data sets. In Section 3.3.2, we showed how to include an interaction term in the regression model in order to accommodate non-additive relationships. A small p-value associated with the interaction term indicates the presence of such relationships. Figure 3.5 suggested that the `Advertising` data may not be additive. Including an interaction term in the model results in a substantial increase in R^2, from around 90 % to almost 97 %.

3.5 Comparison of Linear Regression with K-Nearest Neighbors

As discussed in Chapter 2, linear regression is an example of a *parametric* approach because it assumes a linear functional form for $f(X)$. Parametric methods have several advantages. They are often easy to fit, because one need estimate only a small number of coefficients. In the case of linear regression, the coefficients have simple interpretations, and tests of statistical significance can be easily performed. But parametric methods do have a disadvantage: by construction, they make strong assumptions about the form of $f(X)$. If the specified functional form is far from the truth, and prediction accuracy is our goal, then the parametric method will perform poorly. For instance, if we assume a linear relationship between X and Y but the true relationship is far from linear, then the resulting model will provide a poor fit to the data, and any conclusions drawn from it will be suspect.

In contrast, *non-parametric* methods do not explicitly assume a parametric form for $f(X)$, and thereby provide an alternative and more flexible approach for performing regression. We discuss various non-parametric methods in this book. Here we consider one of the simplest and best-known non-parametric methods, *K-nearest neighbors regression* (KNN regression). The KNN regression method is closely related to the KNN classifier discussed in Chapter 2. Given a value for K and a prediction point x_0, KNN regression first identifies the K training observations that are closest to x_0, represented by $\mathcal{N}_0$. It then estimates $f(x_0)$ using the average of all the

K-nearest neighbors regression

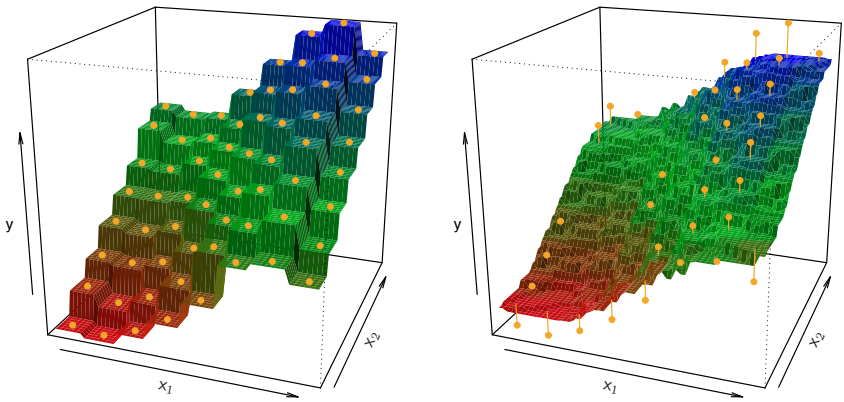


FIGURE 3.16. *Plots of $\hat{f}(X)$ using KNN regression on a two-dimensional data set with 64 observations (orange dots).* Left: $K = 1$ *results in a rough step function fit.* Right: $K = 9$ *produces a much smoother fit.*

training responses in $\mathcal{N}_0$. In other words,

$$\hat{f}(x_0) = \frac{1}{K} \sum_{x_i \in \mathcal{N}_0} y_i.$$

Figure 3.16 illustrates two KNN fits on a data set with $p = 2$ predictors. The fit with $K = 1$ is shown in the left-hand panel, while the right-hand panel corresponds to $K = 9$. We see that when $K = 1$, the KNN fit perfectly interpolates the training observations, and consequently takes the form of a step function. When $K = 9$, the KNN fit still is a step function, but averaging over nine observations results in much smaller regions of constant prediction, and consequently a smoother fit. In general, the optimal value for K will depend on the *bias-variance tradeoff*, which we introduced in Chapter 2. A small value for K provides the most flexible fit, which will have low bias but high variance. This variance is due to the fact that the prediction in a given region is entirely dependent on just one observation. In contrast, larger values of K provide a smoother and less variable fit; the prediction in a region is an average of several points, and so changing one observation has a smaller effect. However, the smoothing may cause bias by masking some of the structure in $f(X)$. In Chapter 5, we introduce several approaches for estimating test error rates. These methods can be used to identify the optimal value of K in KNN regression.

In what setting will a parametric approach such as least squares linear regression outperform a non-parametric approach such as KNN regression? The answer is simple: *the parametric approach will outperform the non-parametric approach if the parametric form that has been selected is close to the true form of f*. Figure 3.17 provides an example with data generated

from a one-dimensional linear regression model. The black solid lines represent $f(X)$, while the blue curves correspond to the KNN fits using $K = 1$ and $K = 9$. In this case, the $K = 1$ predictions are far too variable, while the smoother $K = 9$ fit is much closer to $f(X)$. However, since the true relationship is linear, it is hard for a non-parametric approach to compete with linear regression: a non-parametric approach incurs a cost in variance that is not offset by a reduction in bias. The blue dashed line in the left-hand panel of Figure 3.18 represents the linear regression fit to the same data. It is almost perfect. The right-hand panel of Figure 3.18 reveals that linear regression outperforms KNN for this data. The green solid line, plotted as a function of $1/K$, represents the test set mean squared error (MSE) for KNN. The KNN errors are well above the black dashed line, which is the test MSE for linear regression. When the value of K is large, then KNN performs only a little worse than least squares regression in terms of MSE. It performs far worse when K is small.

In practice, the true relationship between X and Y is rarely exactly linear. Figure 3.19 examines the relative performances of least squares regression and KNN under increasing levels of non-linearity in the relationship between X and Y. In the top row, the true relationship is nearly linear. In this case we see that the test MSE for linear regression is still superior to that of KNN for low values of K. However, for $K \geq 4$, KNN outperforms linear regression. The second row illustrates a more substantial deviation from linearity. In this situation, KNN substantially outperforms linear regression for all values of K. Note that as the extent of non-linearity increases, there is little change in the test set MSE for the non-parametric KNN method, but there is a large increase in the test set MSE of linear regression.

Figures 3.18 and 3.19 display situations in which KNN performs slightly worse than linear regression when the relationship is linear, but much better than linear regression for nonlinear situations. In a real life situation in which the true relationship is unknown, one might suspect that KNN should be favored over linear regression because it will at worst be slightly inferior to linear regression if the true relationship is linear, and may give substantially better results if the true relationship is non-linear. But in reality, even when the true relationship is highly non-linear, KNN may still provide inferior results to linear regression. In particular, both Figures 3.18 and 3.19 illustrate settings with $p = 1$ predictor. But in higher dimensions, KNN often performs worse than linear regression.

Figure 3.20 considers the same strongly non-linear situation as in the second row of Figure 3.19, except that we have added additional *noise* predictors that are not associated with the response. When $p = 1$ or $p = 2$, KNN outperforms linear regression. But for $p = 3$ the results are mixed, and for $p \geq 4$ linear regression is superior to KNN. In fact, the increase in dimension has only caused a small deterioration in the linear regression test set MSE, but it has caused more than a ten-fold increase in the MSE for

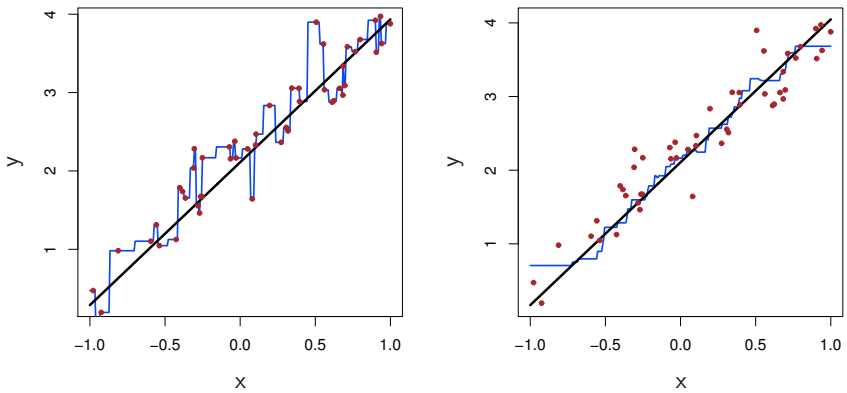


FIGURE 3.17. *Plots of $\hat{f}(X)$ using KNN regression on a one-dimensional data set with 50 observations. The true relationship is given by the black solid line.* Left: *The blue curve corresponds to $K = 1$ and interpolates (i.e. passes directly through) the training data.* Right: *The blue curve corresponds to $K = 9$, and represents a smoother fit.*

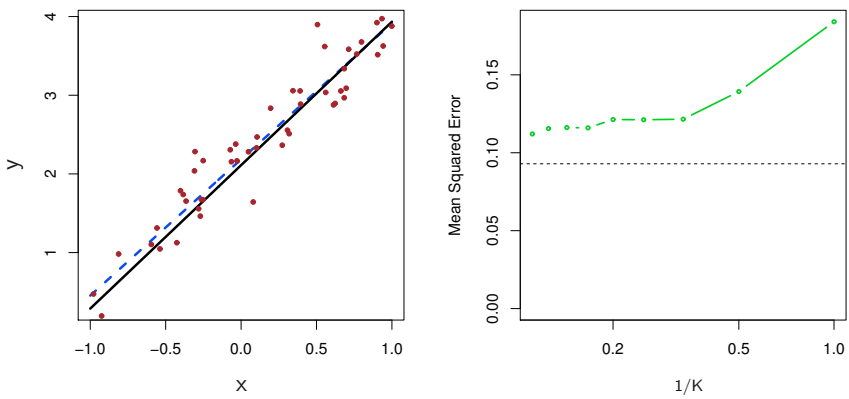


FIGURE 3.18. *The same data set shown in Figure 3.17 is investigated further.* Left: *The blue dashed line is the least squares fit to the data. Since $f(X)$ is in fact linear (displayed as the black line), the least squares regression line provides a very good estimate of $f(X)$.* Right: *The dashed horizontal line represents the least squares test set MSE, while the green solid line corresponds to the MSE for KNN as a function of $1/K$ (on the log scale). Linear regression achieves a lower test MSE than does KNN regression, since $f(X)$ is in fact linear. For KNN regression, the best results occur with a very large value of K, corresponding to a small value of $1/K$.*

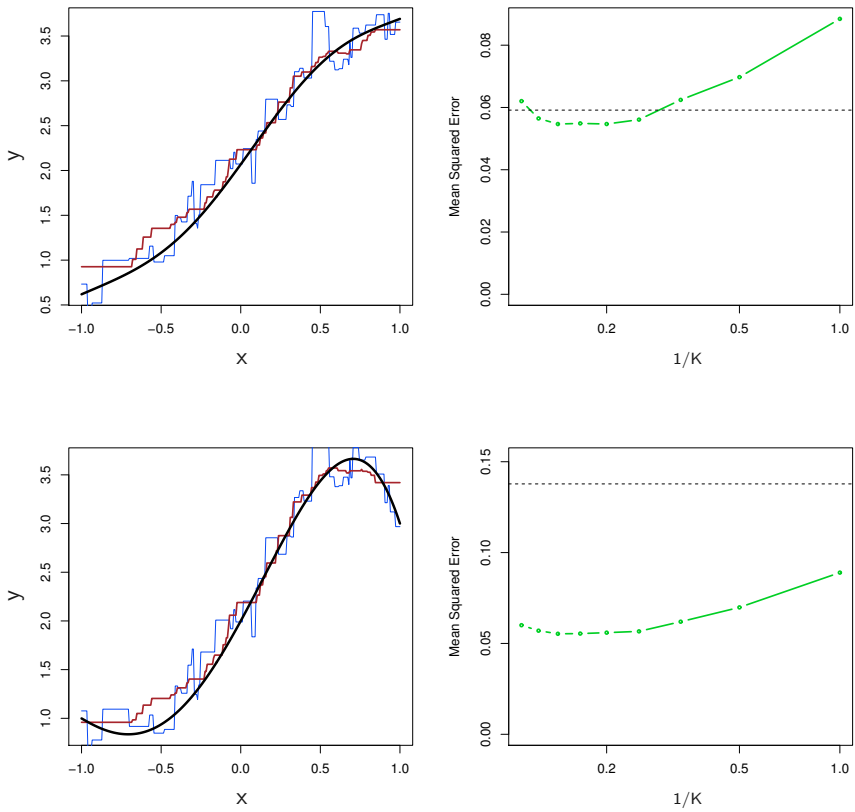


FIGURE 3.19. Top Left: *In a setting with a slightly non-linear relationship between X and Y (solid black line), the KNN fits with $K = 1$ (blue) and $K = 9$ (red) are displayed.* Top Right: *For the slightly non-linear data, the test set MSE for least squares regression (horizontal black) and KNN with various values of $1/K$ (green) are displayed.* Bottom Left and Bottom Right: *As in the top panel, but with a strongly non-linear relationship between X and Y.*

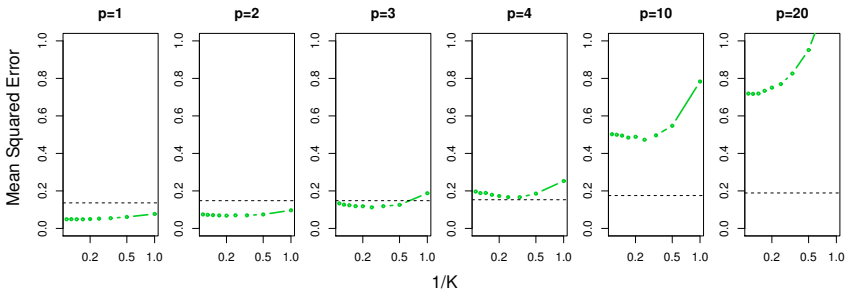


FIGURE 3.20. *Test MSE for linear regression (black dashed lines) and KNN (green curves) as the number of variables p increases. The true function is nonlinear in the first variable, as in the lower panel in Figure 3.19, and does not depend on the additional variables. The performance of linear regression deteriorates slowly in the presence of these additional noise variables, whereas KNN's performance degrades much more quickly as p increases.*

KNN. This decrease in performance as the dimension increases is a common problem for KNN, and results from the fact that in higher dimensions there is effectively a reduction in sample size. In this data set there are 50 training observations; when $p = 1$, this provides enough information to accurately estimate $f(X)$. However, spreading 50 observations over $p = 20$ dimensions results in a phenomenon in which a given observation has no *nearby neighbors*—this is the so-called *curse of dimensionality*. That is, the K observations that are nearest to a given test observation x_0 may be very far away from x_0 in p-dimensional space when p is large, leading to a very poor prediction of $f(x_0)$ and hence a poor KNN fit. As a general rule, parametric methods will tend to outperform non-parametric approaches when there is a small number of observations per predictor.

curse of dimensionality

Even when the dimension is small, we might prefer linear regression to KNN from an interpretability standpoint. If the test MSE of KNN is only slightly lower than that of linear regression, we might be willing to forego a little bit of prediction accuracy for the sake of a simple model that can be described in terms of just a few coefficients, and for which p-values are available.

3.6 Lab: Linear Regression

3.6.1 Libraries

The `library()` function is used to load *libraries*, or groups of functions and data sets that are not included in the base `R` distribution. Basic functions that perform least squares linear regression and other simple analyses come standard with the base distribution, but more exotic functions require

`library()`

additional libraries. Here we load the MASS package, which is a very large collection of data sets and functions. We also load the ISLR2 package, which includes the data sets associated with this book.

```
> library(MASS)
> library(ISLR2)
```

If you receive an error message when loading any of these libraries, it likely indicates that the corresponding library has not yet been installed on your system. Some libraries, such as MASS, come with R and do not need to be separately installed on your computer. However, other packages, such as ISLR2, must be downloaded the first time they are used. This can be done directly from within R. For example, on a Windows system, select the Install package option under the Packages tab. After you select any mirror site, a list of available packages will appear. Simply select the package you wish to install and R will automatically download the package. Alternatively, this can be done at the R command line via install.packages("ISLR2"). This installation only needs to be done the first time you use a package. However, the library() function must be called within each R session.

3.6.2 Simple Linear Regression

The ISLR2 library contains the Boston data set, which records medv (median house value) for 506 census tracts in Boston. We will seek to predict medv using 12 predictors such as rm (average number of rooms per house), age (proportion of owner-occupied units built prior to 1940), and lstat (percent of households with low socioeconomic status).

```
> head(Boston)
     crim zn indus chas   nox    rm  age    dis rad tax
1 0.00632 18  2.31    0 0.538 6.575 65.2 4.0900   1 296
2 0.02731  0  7.07    0 0.469 6.421 78.9 4.9671   2 242
3 0.02729  0  7.07    0 0.469 7.185 61.1 4.9671   2 242
4 0.03237  0  2.18    0 0.458 6.998 45.8 6.0622   3 222
5 0.06905  0  2.18    0 0.458 7.147 54.2 6.0622   3 222
6 0.02985  0  2.18    0 0.458 6.430 58.7 6.0622   3 222
  ptratio lstat medv
1    15.3  4.98 24.0
2    17.8  9.14 21.6
3    17.8  4.03 34.7
4    18.7  2.94 33.4
5    18.7  5.33 36.2
6    18.7  5.21 28.7
```

To find out more about the data set, we can type ?Boston.

We will start by using the lm() function to fit a simple linear regression model, with medv as the response and lstat as the predictor. The basic syntax is lm(y ∼ x, data), where y is the response, x is the predictor, and data is the data set in which these two variables are kept.

lm()

```
> lm.fit <- lm(medv ~ lstat)
Error in eval(expr, envir, enclos) : Object "medv" not found
```

The command causes an error because R does not know where to find the variables medv and lstat. The next line tells R that the variables are in Boston. If we attach Boston, the first line works fine because R now recognizes the variables.

```
> lm.fit <- lm(medv ~ lstat, data = Boston)
> attach(Boston)
> lm.fit <- lm(medv ~ lstat)
```

If we type lm.fit, some basic information about the model is output. For more detailed information, we use summary(lm.fit). This gives us p-values and standard errors for the coefficients, as well as the R^2 statistic and F-statistic for the model.

```
> lm.fit

Call:
lm(formula = medv ~ lstat)

Coefficients:
(Intercept)        lstat
      34.55        -0.95

> summary(lm.fit)

Call:
lm(formula = medv ~ lstat)

Residuals:
   Min     1Q Median     3Q    Max
-15.17  -3.99  -1.32   2.03  24.50

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  34.5538     0.5626    61.4   <2e-16 ***
lstat        -0.9500     0.0387   -24.5   <2e-16 ***
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1

Residual standard error: 6.22 on 504 degrees of freedom
Multiple R-squared: 0.544,      Adjusted R-squared: 0.543
F-statistic:  602 on 1 and 504 DF,  p-value: < 2e-16
```

We can use the names() function in order to find out what other pieces of information are stored in lm.fit. Although we can extract these quantities by name—e.g. lm.fit$coefficients—it is safer to use the extractor functions like coef() to access them.

names()

coef()

```
> names(lm.fit)
 [1] "coefficients"  "residuals"     "effects"
 [4] "rank"          "fitted.values" "assign"
```

```
 [7] "qr"            "df.residual"   "xlevels"
[10] "call"          "terms"         "model"
> coef(lm.fit)
(Intercept)       lstat
      34.55       -0.95
```

In order to obtain a confidence interval for the coefficient estimates, we can use the `confint()` command.

`confint()`

```
> confint(lm.fit)
             2.5 % 97.5 %
(Intercept) 33.45 35.659
lstat       -1.03 -0.874
```

The `predict()` function can be used to produce confidence intervals and prediction intervals for the prediction of `medv` for a given value of `lstat`.

`predict()`

```
> predict(lm.fit, data.frame(lstat = (c(5, 10, 15))),
    interval = "confidence")
    fit   lwr   upr
1 29.80 29.01 30.60
2 25.05 24.47 25.63
3 20.30 19.73 20.87
> predict(lm.fit, data.frame(lstat = (c(5, 10, 15))),
    interval = "prediction")
    fit    lwr   upr
1 29.80 17.566 42.04
2 25.05 12.828 37.28
3 20.30  8.078 32.53
```

For instance, the 95 % confidence interval associated with a `lstat` value of 10 is $(24.47, 25.63)$, and the 95 % prediction interval is $(12.828, 37.28)$. As expected, the confidence and prediction intervals are centered around the same point (a predicted value of 25.05 for `medv` when `lstat` equals 10), but the latter are substantially wider.

We will now plot `medv` and `lstat` along with the least squares regression line using the `plot()` and `abline()` functions.

`abline()`

```
> plot(lstat, medv)
> abline(lm.fit)
```

There is some evidence for non-linearity in the relationship between `lstat` and `medv`. We will explore this issue later in this lab.

The `abline()` function can be used to draw any line, not just the least squares regression line. To draw a line with intercept `a` and slope `b`, we type `abline(a, b)`. Below we experiment with some additional settings for plotting lines and points. The `lwd = 3` command causes the width of the regression line to be increased by a factor of 3; this works for the `plot()` and `lines()` functions also. We can also use the `pch` option to create different plotting symbols.

```
> abline(lm.fit, lwd = 3)
> abline(lm.fit, lwd = 3, col = "red")
```

```
> plot(lstat, medv, col = "red")
> plot(lstat, medv, pch = 20)
> plot(lstat, medv, pch = "+")
> plot(1:20, 1:20, pch = 1:20)
```

Next we examine some diagnostic plots, several of which were discussed in Section 3.3.3. Four diagnostic plots are automatically produced by applying the `plot()` function directly to the output from `lm()`. In general, this command will produce one plot at a time, and hitting *Enter* will generate the next plot. However, it is often convenient to view all four plots together. We can achieve this by using the `par()` and `mfrow()` functions, which tell R to split the display screen into separate panels so that multiple plots can be viewed simultaneously. For example, `par(mfrow = c(2, 2))` divides the plotting region into a 2×2 grid of panels.

`par()`
`mfrow()`

```
> par(mfrow = c(2, 2))
> plot(lm.fit)
```

Alternatively, we can compute the residuals from a linear regression fit using the `residuals()` function. The function `rstudent()` will return the studentized residuals, and we can use this function to plot the residuals against the fitted values.

`residuals()`
`rstudent()`

```
> plot(predict(lm.fit), residuals(lm.fit))
> plot(predict(lm.fit), rstudent(lm.fit))
```

On the basis of the residual plots, there is some evidence of non-linearity. Leverage statistics can be computed for any number of predictors using the `hatvalues()` function.

`hatvalues()`

```
> plot(hatvalues(lm.fit))
> which.max(hatvalues(lm.fit))
375
```

The `which.max()` function identifies the index of the largest element of a vector. In this case, it tells us which observation has the largest leverage statistic.

`which.max()`

3.6.3 Multiple Linear Regression

In order to fit a multiple linear regression model using least squares, we again use the `lm()` function. The syntax `lm(y ~ x1 + x2 + x3)` is used to fit a model with three predictors, `x1`, `x2`, and `x3`. The `summary()` function now outputs the regression coefficients for all the predictors.

```
> lm.fit <- lm(medv ~ lstat + age, data = Boston)
> summary(lm.fit)

Call:
lm(formula = medv ~ lstat + age, data = Boston)

Residuals:
```

```
   Min     1Q Median     3Q    Max
-15.98  -3.98  -1.28   1.97  23.16

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  33.2228     0.7308   45.46   <2e-16 ***
lstat        -1.0321     0.0482  -21.42   <2e-16 ***
age           0.0345     0.0122    2.83   0.0049 **
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1  1

Residual standard error: 6.17 on 503 degrees of freedom
Multiple R-squared: 0.551,      Adjusted R-squared: 0.549
F-statistic:  309 on 2 and 503 DF,  p-value: < 2e-16
```

The `Boston` data set contains 12 variables, and so it would be cumbersome to have to type all of these in order to perform a regression using all of the predictors. Instead, we can use the following short-hand:

```
> lm.fit <- lm(medv ~ ., data = Boston)
> summary(lm.fit)

Call:
lm(formula = medv ~ ., data = Boston)

Residuals:
    Min      1Q  Median      3Q     Max
-15.130  -2.767  -0.581   1.941  26.253

Coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept)  41.61727    4.93604    8.43  3.8e-16 ***
crim         -0.12139    0.03300   -3.68  0.00026 ***
zn            0.04696    0.01388    3.38  0.00077 ***
indus         0.01347    0.06214    0.22  0.82852
chas          2.83999    0.87001    3.26  0.00117 **
nox         -18.75802    3.85135   -4.87  1.5e-06 ***
rm            3.65812    0.42025    8.70  < 2e-16 ***
age           0.00361    0.01333    0.27  0.78659
dis          -1.49075    0.20162   -7.39  6.2e-13 ***
rad           0.28940    0.06691    4.33  1.8e-05 ***
tax          -0.01268    0.00380   -3.34  0.00091 ***
ptratio      -0.93753    0.13221   -7.09  4.6e-12 ***
lstat        -0.55202    0.05066  -10.90  < 2e-16 ***
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1

Residual standard error: 4.8 on 493 degrees of freedom
Multiple R-squared:  0.734,     Adjusted R-squared:  0.728
F-statistic:  114 on 12 and 493 DF,  p-value: < 2e-16
```

We can access the individual components of a summary object by name (type `?summary.lm` to see what is available). Hence `summary(lm.fit)$r.sq` gives us the R^2, and `summary(lm.fit)$sigma` gives us the RSE. The `vif()`

`vif()`

function, part of the car package, can be used to compute variance inflation factors. Most VIF's are low to moderate for this data. The car package is not part of the base R installation so it must be downloaded the first time you use it via the install.packages() function in R.

```
> library(car)
> vif(lm.fit)
   crim      zn   indus    chas     nox      rm     age     dis
   1.77    2.30    3.99    1.07    4.37    1.91    3.09    3.95
    rad     tax ptratio   lstat
   7.45    9.00    1.80    2.87
```

What if we would like to perform a regression using all of the variables but one? For example, in the above regression output, age has a high p-value. So we may wish to run a regression excluding this predictor. The following syntax results in a regression using all predictors except age.

```
> lm.fit1 <- lm(medv ~ . - age, data = Boston)
> summary(lm.fit1)
...
```

Alternatively, the update() function can be used.

update()

```
> lm.fit1 <- update(lm.fit, ~ . - age)
```

3.6.4 Interaction Terms

It is easy to include interaction terms in a linear model using the lm() function. The syntax lstat:age tells R to include an interaction term between lstat and age. The syntax lstat * age simultaneously includes lstat, age, and the interaction term lstat×age as predictors; it is a shorthand for lstat + age + lstat:age.

```
> summary(lm(medv ~ lstat * age, data = Boston))

Call:
lm(formula = medv ~ lstat * age, data = Boston)

Residuals:
    Min      1Q  Median      3Q     Max
-15.81  -4.04  -1.33    2.08  27.55

Coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept) 36.088536   1.469835   24.55  < 2e-16 ***
lstat       -1.392117   0.167456   -8.31  8.8e-16 ***
age         -0.000721   0.019879   -0.04    0.971
lstat:age    0.004156   0.001852    2.24    0.025 *
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1

Residual standard error: 6.15 on 502 degrees of freedom
```

```
Multiple R-squared: 0.556,  Adjusted R-squared: 0.553
F-statistic:  209 on 3 and 502 DF,  p-value: < 2e-16
```

3.6.5 Non-linear Transformations of the Predictors

The `lm()` function can also accommodate non-linear transformations of the predictors. For instance, given a predictor X, we can create a predictor X^2 using `I(X^2)`. The function `I()` is needed since the `^` has a special meaning in a formula object; wrapping as we do allows the standard usage in `R`, which is to raise `X` to the power `2`. We now perform a regression of `medv` onto `lstat` and `lstat`^{2}.

`I()`

```
> lm.fit2 <- lm(medv ~ lstat + I(lstat^2))
> summary(lm.fit2)

Call:
lm(formula = medv ~ lstat + I(lstat^2))

Residuals:
   Min     1Q Median     3Q    Max
-15.28  -3.83  -0.53   2.31  25.41

Coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept) 42.86201    0.87208    49.1   <2e-16 ***
lstat       -2.33282    0.12380   -18.8   <2e-16 ***
I(lstat^2)   0.04355    0.00375    11.6   <2e-16 ***
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1

Residual standard error: 5.52 on 503 degrees of freedom
Multiple R-squared: 0.641,  Adjusted R-squared: 0.639
F-statistic:  449 on 2 and 503 DF,  p-value: < 2e-16
```

The near-zero p-value associated with the quadratic term suggests that it leads to an improved model. We use the `anova()` function to further quantify the extent to which the quadratic fit is superior to the linear fit.

`anova()`

```
> lm.fit <- lm(medv ~ lstat)
> anova(lm.fit, lm.fit2)
Analysis of Variance Table

Model 1: medv ~ lstat
Model 2: medv ~ lstat + I(lstat^2)
  Res.Df   RSS Df Sum of Sq   F Pr(>F)
1    504 19472
2    503 15347  1      4125 135 <2e-16 ***
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1
```

Here Model 1 represents the linear submodel containing only one predictor, `lstat`, while Model 2 corresponds to the larger quadratic model that has two

predictors, lstat and $\texttt{lstat}^2$. The anova() function performs a hypothesis test comparing the two models. The null hypothesis is that the two models fit the data equally well, and the alternative hypothesis is that the full model is superior. Here the F-statistic is 135 and the associated p-value is virtually zero. This provides very clear evidence that the model containing the predictors lstat and $\texttt{lstat}^2$ is far superior to the model that only contains the predictor lstat. This is not surprising, since earlier we saw evidence for non-linearity in the relationship between medv and lstat. If we type

```
> par(mfrow = c(2, 2))
> plot(lm.fit2)
```

then we see that when the $\texttt{lstat}^2$ term is included in the model, there is little discernible pattern in the residuals.

In order to create a cubic fit, we can include a predictor of the form I(X^3). However, this approach can start to get cumbersome for higher-order polynomials. A better approach involves using the poly() function to create the polynomial within lm(). For example, the following command produces a fifth-order polynomial fit:

poly()

```
> lm.fit5 <- lm(medv ~ poly(lstat, 5))
> summary(lm.fit5)

Call:
lm(formula = medv ~ poly(lstat, 5))

Residuals:
    Min      1Q  Median      3Q     Max
-13.543  -3.104  -0.705   2.084  27.115

Coefficients:
                Estimate Std. Error t value Pr(>|t|)
(Intercept)       22.533      0.232   97.20  < 2e-16 ***
poly(lstat, 5)1 -152.460      5.215  -29.24  < 2e-16 ***
poly(lstat, 5)2   64.227      5.215   12.32  < 2e-16 ***
poly(lstat, 5)3  -27.051      5.215   -5.19  3.1e-07 ***
poly(lstat, 5)4   25.452      5.215    4.88  1.4e-06 ***
poly(lstat, 5)5  -19.252      5.215   -3.69  0.00025 ***
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1

Residual standard error: 5.21 on 500 degrees of freedom
Multiple R-squared: 0.682,  Adjusted R-squared: 0.679
F-statistic:  214 on 5 and 500 DF,  p-value: < 2e-16
```

This suggests that including additional polynomial terms, up to fifth order, leads to an improvement in the model fit! However, further investigation of the data reveals that no polynomial terms beyond fifth order have significant p-values in a regression fit.

By default, the poly() function orthogonalizes the predictors: this means that the features output by this function are not simply a sequence of

powers of the argument. However, a linear model applied to the output of the `poly()` function will have the same fitted values as a linear model applied to the raw polynomials (although the coefficient estimates, standard errors, and p-values will differ). In order to obtain the raw polynomials from the `poly()` function, the argument `raw = TRUE` must be used.

Of course, we are in no way restricted to using polynomial transformations of the predictors. Here we try a log transformation.

```
> summary(lm(medv ~ log(rm), data = Boston))
...
```

3.6.6 Qualitative Predictors

We will now examine the `Carseats` data, which is part of the `ISLR2` library. We will attempt to predict `Sales` (child car seat sales) in 400 locations based on a number of predictors.

```
> head(Carseats)
  Sales CompPrice Income Advertising Population Price
1  9.50       138     73          11        276   120
2 11.22       111     48          16        260    83
3 10.06       113     35          10        269    80
4  7.40       117    100           4        466    97
5  4.15       141     64           3        340   128
6 10.81       124    113          13        501    72
  ShelveLoc Age Education Urban  US
1       Bad  42        17   Yes Yes
2      Good  65        10   Yes Yes
3    Medium  59        12   Yes Yes
4    Medium  55        14   Yes Yes
5       Bad  38        13   Yes  No
6       Bad  78        16    No Yes
```

The `Carseats` data includes qualitative predictors such as `Shelveloc`, an indicator of the quality of the shelving location—that is, the space within a store in which the car seat is displayed—at each location. The predictor `Shelveloc` takes on three possible values: *Bad*, *Medium*, and *Good*. Given a qualitative variable such as `Shelveloc`, `R` generates dummy variables automatically. Below we fit a multiple regression model that includes some interaction terms.

```
> lm.fit <- lm(Sales ~ . + Income:Advertising + Price:Age,
    data = Carseats)
> summary(lm.fit)

Call:
lm(formula = Sales ~ . + Income:Advertising + Price:Age, data =
Carseats)

Residuals:
   Min     1Q Median     3Q    Max
```

```
-2.921 -0.750  0.018  0.675  3.341

Coefficients:
                    Estimate Std. Error t value Pr(>|t|)
(Intercept)         6.575565   1.008747    6.52  2.2e-10 ***
CompPrice           0.092937   0.004118   22.57  < 2e-16 ***
Income              0.010894   0.002604    4.18  3.6e-05 ***
Advertising         0.070246   0.022609    3.11  0.00203 **
Population          0.000159   0.000368    0.43  0.66533
Price              -0.100806   0.007440  -13.55  < 2e-16 ***
ShelveLocGood       4.848676   0.152838   31.72  < 2e-16 ***
ShelveLocMedium     1.953262   0.125768   15.53  < 2e-16 ***
Age                -0.057947   0.015951   -3.63  0.00032 ***
Education          -0.020852   0.019613   -1.06  0.28836
UrbanYes            0.140160   0.112402    1.25  0.21317
USYes              -0.157557   0.148923   -1.06  0.29073
Income:Advertising  0.000751   0.000278    2.70  0.00729 **
Price:Age           0.000107   0.000133    0.80  0.42381
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1

Residual standard error: 1.01 on 386 degrees of freedom
Multiple R-squared: 0.876,      Adjusted R-squared: 0.872
F-statistic:  210 on 13 and 386 DF,  p-value: < 2e-16
```

The `contrasts()` function returns the coding that `R` uses for the dummy variables. `contrasts()`

```
> attach(Carseats)
> contrasts(ShelveLoc)
       Good Medium
Bad       0      0
Good      1      0
Medium    0      1
```

Use `?contrasts` to learn about other contrasts, and how to set them.

`R` has created a `ShelveLocGood` dummy variable that takes on a value of 1 if the shelving location is good, and 0 otherwise. It has also created a `ShelveLocMedium` dummy variable that equals 1 if the shelving location is medium, and 0 otherwise. A bad shelving location corresponds to a zero for each of the two dummy variables. The fact that the coefficient for `ShelveLocGood` in the regression output is positive indicates that a good shelving location is associated with high sales (relative to a bad location). And `ShelveLocMedium` has a smaller positive coefficient, indicating that a medium shelving location is associated with higher sales than a bad shelving location but lower sales than a good shelving location.

3.6.7 Writing Functions

As we have seen, `R` comes with many useful functions, and still more functions are available by way of `R` libraries. However, we will often be inter-

ested in performing an operation for which no function is available. In this setting, we may want to write our own function. For instance, below we provide a simple function that reads in the ISLR2 and MASS libraries, called LoadLibraries(). Before we have created the function, R returns an error if we try to call it.

```
> LoadLibraries
Error: object `LoadLibraries' not found
> LoadLibraries()
Error: could not find function "LoadLibraries"
```

We now create the function. Note that the + symbols are printed by R and should not be typed in. The { symbol informs R that multiple commands are about to be input. Hitting *Enter* after typing { will cause R to print the + symbol. We can then input as many commands as we wish, hitting *Enter* after each one. Finally the } symbol informs R that no further commands will be entered.

```
> LoadLibraries <- function() {
+   library(ISLR2)
+   library(MASS)
+   print("The libraries have been loaded.")
+ }
```

Now if we type in LoadLibraries, R will tell us what is in the function.

```
> LoadLibraries
function() {
  library(ISLR2)
  library(MASS)
  print("The libraries have been loaded.")
}
```

If we call the function, the libraries are loaded in and the print statement is output.

```
> LoadLibraries()
[1] "The libraries have been loaded."
```

3.7 Exercises

Conceptual

1. Describe the null hypotheses to which the p-values given in Table 3.4 correspond. Explain what conclusions you can draw based on these p-values. Your explanation should be phrased in terms of sales, TV, radio, and newspaper, rather than in terms of the coefficients of the linear model.

2. Carefully explain the differences between the KNN classifier and KNN regression methods.

3. Suppose we have a data set with five predictors, X_1 = GPA, X_2 = IQ, X_3 = Level (1 for College and 0 for High School), X_4 = Interaction between GPA and IQ, and X_5 = Interaction between GPA and Level. The response is starting salary after graduation (in thousands of dollars). Suppose we use least squares to fit the model, and get $\hat{\beta}_0 = 50, \hat{\beta}_1 = 20, \hat{\beta}_2 = 0.07, \hat{\beta}_3 = 35, \hat{\beta}_4 = 0.01, \hat{\beta}_5 = -10$.

   (a) Which answer is correct, and why?

      i. For a fixed value of IQ and GPA, high school graduates earn more, on average, than college graduates.

      ii. For a fixed value of IQ and GPA, college graduates earn more, on average, than high school graduates.

      iii. For a fixed value of IQ and GPA, high school graduates earn more, on average, than college graduates provided that the GPA is high enough.

      iv. For a fixed value of IQ and GPA, college graduates earn more, on average, than high school graduates provided that the GPA is high enough.

   (b) Predict the salary of a college graduate with IQ of 110 and a GPA of 4.0.

   (c) True or false: Since the coefficient for the GPA/IQ interaction term is very small, there is very little evidence of an interaction effect. Justify your answer.

4. I collect a set of data ($n = 100$ observations) containing a single predictor and a quantitative response. I then fit a linear regression model to the data, as well as a separate cubic regression, i.e. $Y = \beta_0 + \beta_1 X + \beta_2 X^2 + \beta_3 X^3 + \epsilon$.

   (a) Suppose that the true relationship between X and Y is linear, i.e. $Y = \beta_0 + \beta_1 X + \epsilon$. Consider the training residual sum of squares (RSS) for the linear regression, and also the training RSS for the cubic regression. Would we expect one to be lower than the other, would we expect them to be the same, or is there not enough information to tell? Justify your answer.

   (b) Answer (a) using test rather than training RSS.

   (c) Suppose that the true relationship between X and Y is not linear, but we don't know how far it is from linear. Consider the training RSS for the linear regression, and also the training RSS for the cubic regression. Would we expect one to be lower than the other, would we expect them to be the same, or is there not enough information to tell? Justify your answer.

   (d) Answer (c) using test rather than training RSS.

5. Consider the fitted values that result from performing linear regression without an intercept. In this setting, the ith fitted value takes the form

$$\hat{y}_i = x_i\hat{\beta},$$

where

$$\hat{\beta} = \left(\sum_{i=1}^{n} x_i y_i\right) / \left(\sum_{i'=1}^{n} x_{i'}^2\right). \tag{3.38}$$

Show that we can write

$$\hat{y}_i = \sum_{i'=1}^{n} a_{i'} y_{i'}.$$

What is $a_{i'}$?

Note: We interpret this result by saying that the fitted values from linear regression are linear combinations *of the response values.*

6. Using (3.4), argue that in the case of simple linear regression, the least squares line always passes through the point $(\bar{x}, \bar{y})$.

7. It is claimed in the text that in the case of simple linear regression of Y onto X, the R^2 statistic (3.17) is equal to the square of the correlation between X and Y (3.18). Prove that this is the case. For simplicity, you may assume that $\bar{x} = \bar{y} = 0$.

Applied

8. This question involves the use of simple linear regression on the `Auto` data set.

   (a) Use the `lm()` function to perform a simple linear regression with `mpg` as the response and `horsepower` as the predictor. Use the `summary()` function to print the results. Comment on the output. For example:

      i. Is there a relationship between the predictor and the response?
      ii. How strong is the relationship between the predictor and the response?
      iii. Is the relationship between the predictor and the response positive or negative?
      iv. What is the predicted `mpg` associated with a `horsepower` of 98? What are the associated 95 % confidence and prediction intervals?

(b) Plot the response and the predictor. Use the `abline()` function to display the least squares regression line.

(c) Use the `plot()` function to produce diagnostic plots of the least squares regression fit. Comment on any problems you see with the fit.

9. This question involves the use of multiple linear regression on the `Auto` data set.

(a) Produce a scatterplot matrix which includes all of the variables in the data set.

(b) Compute the matrix of correlations between the variables using the function `cor()`. You will need to exclude the `name` variable, which is qualitative. `cor()`

(c) Use the `lm()` function to perform a multiple linear regression with `mpg` as the response and all other variables except `name` as the predictors. Use the `summary()` function to print the results. Comment on the output. For instance:

i. Is there a relationship between the predictors and the response?

ii. Which predictors appear to have a statistically significant relationship to the response?

iii. What does the coefficient for the `year` variable suggest?

(d) Use the `plot()` function to produce diagnostic plots of the linear regression fit. Comment on any problems you see with the fit. Do the residual plots suggest any unusually large outliers? Does the leverage plot identify any observations with unusually high leverage?

(e) Use the `*` and `:` symbols to fit linear regression models with interaction effects. Do any interactions appear to be statistically significant?

(f) Try a few different transformations of the variables, such as $\log(X)$, $\sqrt{X}$, X^2. Comment on your findings.

10. This question should be answered using the `Carseats` data set.

(a) Fit a multiple regression model to predict `Sales` using `Price`, `Urban`, and `US`.

(b) Provide an interpretation of each coefficient in the model. Be careful—some of the variables in the model are qualitative!

(c) Write out the model in equation form, being careful to handle the qualitative variables properly.

(d) For which of the predictors can you reject the null hypothesis $H_0 : \beta_j = 0$?

(e) On the basis of your response to the previous question, fit a smaller model that only uses the predictors for which there is evidence of association with the outcome.

(f) How well do the models in (a) and (e) fit the data?

(g) Using the model from (e), obtain 95 % confidence intervals for the coefficient(s).

(h) Is there evidence of outliers or high leverage observations in the model from (e)?

11. In this problem we will investigate the t-statistic for the null hypothesis $H_0 : \beta = 0$ in simple linear regression without an intercept. To begin, we generate a predictor `x` and a response `y` as follows.

```
> set.seed(1)
> x <- rnorm(100)
> y <- 2 * x + rnorm(100)
```

(a) Perform a simple linear regression of `y` onto `x`, *without* an intercept. Report the coefficient estimate $\hat{\beta}$, the standard error of this coefficient estimate, and the t-statistic and p-value associated with the null hypothesis $H_0 : \beta = 0$. Comment on these results. (You can perform regression without an intercept using the command `lm(y~x+0)`.)

(b) Now perform a simple linear regression of `x` onto `y` without an intercept, and report the coefficient estimate, its standard error, and the corresponding t-statistic and p-values associated with the null hypothesis $H_0 : \beta = 0$. Comment on these results.

(c) What is the relationship between the results obtained in (a) and (b)?

(d) For the regression of Y onto X without an intercept, the t-statistic for $H_0 : \beta = 0$ takes the form $\hat{\beta}/\mathrm{SE}(\hat{\beta})$, where $\hat{\beta}$ is given by (3.38), and where

$$\mathrm{SE}(\hat{\beta}) = \sqrt{\frac{\sum_{i=1}^{n}(y_i - x_i\hat{\beta})^2}{(n-1)\sum_{i'=1}^{n} x_{i'}^2}}.$$

(These formulas are slightly different from those given in Sections 3.1.1 and 3.1.2, since here we are performing regression without an intercept.) Show algebraically, and confirm numerically in `R`, that the t-statistic can be written as

$$\frac{(\sqrt{n-1})\sum_{i=1}^{n} x_i y_i}{\sqrt{(\sum_{i=1}^{n} x_i^2)(\sum_{i'=1}^{n} y_{i'}^2) - (\sum_{i'=1}^{n} x_{i'} y_{i'})^2}}.$$

(e) Using the results from (d), argue that the t-statistic for the regression of `y` onto `x` is the same as the t-statistic for the regression of `x` onto `y`.

(f) In `R`, show that when regression is performed *with* an intercept, the t-statistic for $H_0 : \beta_1 = 0$ is the same for the regression of `y` onto `x` as it is for the regression of `x` onto `y`.

12. This problem involves simple linear regression without an intercept.

(a) Recall that the coefficient estimate $\hat{\beta}$ for the linear regression of Y onto X without an intercept is given by (3.38). Under what circumstance is the coefficient estimate for the regression of X onto Y the same as the coefficient estimate for the regression of Y onto X?

(b) Generate an example in `R` with $n = 100$ observations in which the coefficient estimate for the regression of X onto Y is *different from* the coefficient estimate for the regression of Y onto X.

(c) Generate an example in `R` with $n = 100$ observations in which the coefficient estimate for the regression of X onto Y is *the same as* the coefficient estimate for the regression of Y onto X.

13. In this exercise you will create some simulated data and will fit simple linear regression models to it. Make sure to use `set.seed(1)` prior to starting part (a) to ensure consistent results.

(a) Using the `rnorm()` function, create a vector, `x`, containing 100 observations drawn from a $N(0, 1)$ distribution. This represents a feature, X.

(b) Using the `rnorm()` function, create a vector, `eps`, containing 100 observations drawn from a $N(0, 0.25)$ distribution—a normal distribution with mean zero and variance 0.25.

(c) Using `x` and `eps`, generate a vector `y` according to the model

$$Y = -1 + 0.5X + \epsilon. \tag{3.39}$$

What is the length of the vector `y`? What are the values of β_0 and β_1 in this linear model?

(d) Create a scatterplot displaying the relationship between `x` and `y`. Comment on what you observe.

(e) Fit a least squares linear model to predict `y` using `x`. Comment on the model obtained. How do $\hat{\beta}_0$ and $\hat{\beta}_1$ compare to β_0 and β_1?

(f) Display the least squares line on the scatterplot obtained in (d). Draw the population regression line on the plot, in a different color. Use the `legend()` command to create an appropriate legend.

(g) Now fit a polynomial regression model that predicts `y` using `x` and x^2. Is there evidence that the quadratic term improves the model fit? Explain your answer.

(h) Repeat (a)–(f) after modifying the data generation process in such a way that there is *less* noise in the data. The model (3.39) should remain the same. You can do this by decreasing the variance of the normal distribution used to generate the error term ϵ in (b). Describe your results.

(i) Repeat (a)–(f) after modifying the data generation process in such a way that there is *more* noise in the data. The model (3.39) should remain the same. You can do this by increasing the variance of the normal distribution used to generate the error term ϵ in (b). Describe your results.

(j) What are the confidence intervals for β_0 and β_1 based on the original data set, the noisier data set, and the less noisy data set? Comment on your results.

14. This problem focuses on the *collinearity* problem.

(a) Perform the following commands in `R`:

```
> set.seed(1)
> x1 <- runif(100)
> x2 <- 0.5 * x1 + rnorm(100) / 10
> y <- 2 + 2 * x1 + 0.3 * x2 + rnorm(100)
```

The last line corresponds to creating a linear model in which `y` is a function of `x1` and `x2`. Write out the form of the linear model. What are the regression coefficients?

(b) What is the correlation between `x1` and `x2`? Create a scatterplot displaying the relationship between the variables.

(c) Using this data, fit a least squares regression to predict `y` using `x1` and `x2`. Describe the results obtained. What are $\hat{\beta}_0$, $\hat{\beta}_1$, and $\hat{\beta}_2$? How do these relate to the true β_0, β_1, and β_2? Can you reject the null hypothesis $H_0 : \beta_1 = 0$? How about the null hypothesis $H_0 : \beta_2 = 0$?

(d) Now fit a least squares regression to predict `y` using only `x1`. Comment on your results. Can you reject the null hypothesis $H_0 : \beta_1 = 0$?

(e) Now fit a least squares regression to predict `y` using only `x2`. Comment on your results. Can you reject the null hypothesis $H_0 : \beta_1 = 0$?

(f) Do the results obtained in (c)–(e) contradict each other? Explain your answer.

(g) Now suppose we obtain one additional observation, which was unfortunately mismeasured.

```
> x1 <- c(x1, 0.1)
> x2 <- c(x2, 0.8)
> y <- c(y, 6)
```

Re-fit the linear models from (c) to (e) using this new data. What effect does this new observation have on the each of the models? In each model, is this observation an outlier? A high-leverage point? Both? Explain your answers.

15. This problem involves the `Boston` data set, which we saw in the lab for this chapter. We will now try to predict per capita crime rate using the other variables in this data set. In other words, per capita crime rate is the response, and the other variables are the predictors.

(a) For each predictor, fit a simple linear regression model to predict the response. Describe your results. In which of the models is there a statistically significant association between the predictor and the response? Create some plots to back up your assertions.

(b) Fit a multiple regression model to predict the response using all of the predictors. Describe your results. For which predictors can we reject the null hypothesis $H_0 : \beta_j = 0$?

(c) How do your results from (a) compare to your results from (b)? Create a plot displaying the univariate regression coefficients from (a) on the x-axis, and the multiple regression coefficients from (b) on the y-axis. That is, each predictor is displayed as a single point in the plot. Its coefficient in a simple linear regression model is shown on the x-axis, and its coefficient estimate in the multiple linear regression model is shown on the y-axis.

(d) Is there evidence of non-linear association between any of the predictors and the response? To answer this question, for each predictor X, fit a model of the form

$$Y = \beta_0 + \beta_1 X + \beta_2 X^2 + \beta_3 X^3 + \epsilon.$$

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

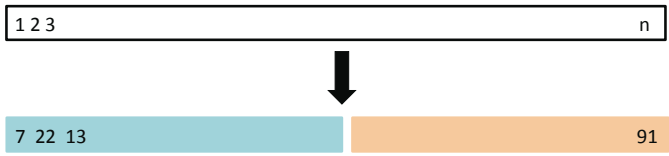


FIGURE 5.1. *A schematic display of the validation set approach. A set of n observations are randomly split into a training set (shown in blue, containing observations 7, 22, and 13, among others) and a validation set (shown in beige, and containing observation 91, among others). The statistical learning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

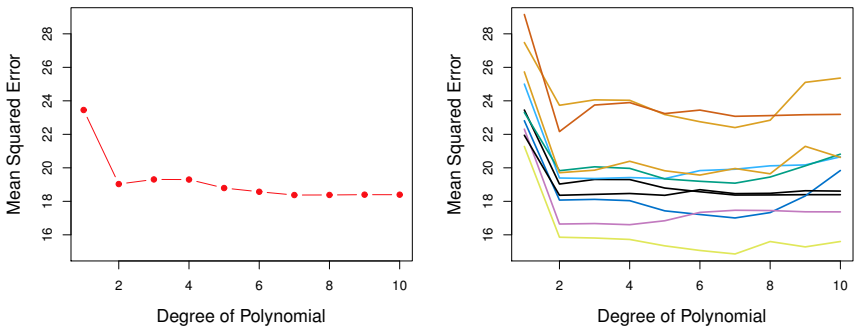


FIGURE 5.2. *The validation set approach was used on the* `Auto` *data set in order to estimate the test error that results from predicting* `mpg` *using polynomial functions of* `horsepower`*.* Left: *Validation error estimates for a single split into training and validation data sets.* Right: *The 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 $\{(x_2, y_2), \ldots, (x_n, y_n)\}$ 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,

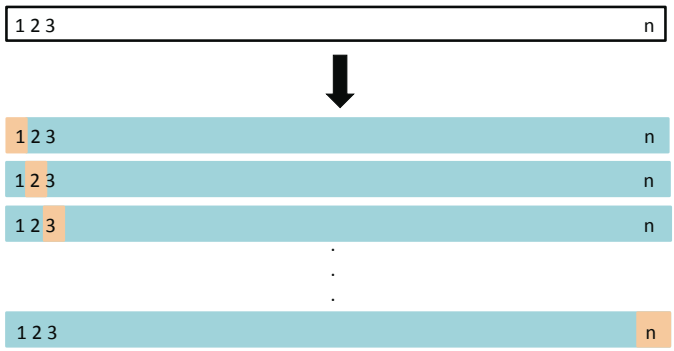


FIGURE 5.3. *A schematic display of LOOCV. A set of n data points is repeatedly split into a training set (shown in blue) containing all but one observation, and a validation set that contains only that observation (shown in beige). The test error is then estimated by averaging the n resulting MSEs.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

using its value x_1. Since (x_1, y_1) was not used in the fitting process, $\text{MSE}_1 = (y_1 - \hat{y}_1)^2$ 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 $\{(x_1, y_1), (x_3, y_3), \ldots, (x_n, y_n)\}$, and computing $\text{MSE}_2 = (y_2 - \hat{y}_2)^2$. Repeating this approach n times produces n squared errors, $\text{MSE}_1, \ldots, \text{MSE}_n$. The LOOCV estimate for the test MSE is the average of these n test error estimates:

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

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

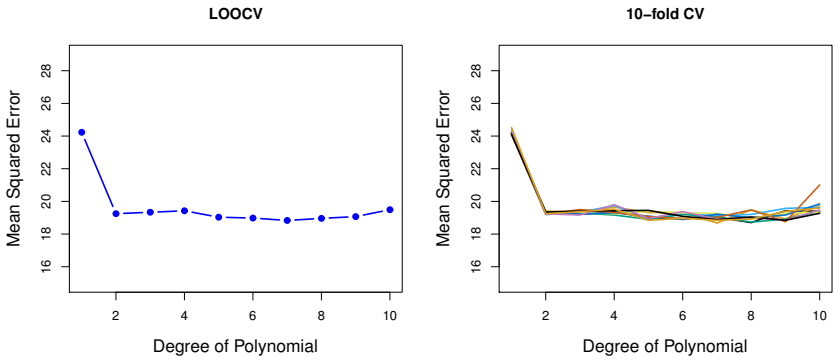


FIGURE 5.4. *Cross-validation was used on the* `Auto` *data set in order to estimate the test error that results from predicting* `mpg` *using polynomial functions of* `horsepower`. Left: *The LOOCV error curve.* Right: 10*-fold CV was run nine separate times, each with a different random split of the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

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

where $\hat{y}_i$ is the ith fitted value from the original least squares fit, and h_i is the leverage defined in (3.37) on page 99.[1] This is like the ordinary MSE, except the ith 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

[1]In the case of multiple linear regression, the leverage takes a slightly more complicated form than (3.37), but (5.2) still holds.

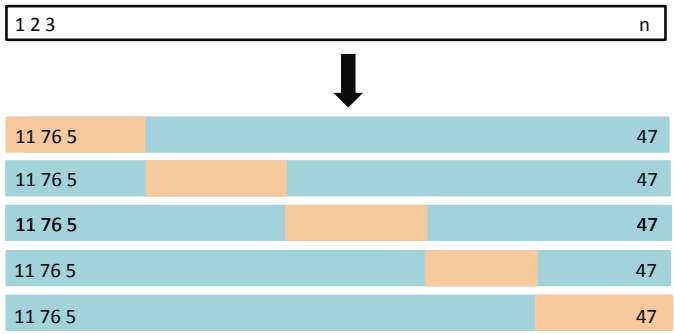


FIGURE 5.5. *A schematic display of 5-fold CV. A set of n observations is randomly split into five non-overlapping groups. Each of these fifths acts as a validation set (shown in beige), and the remainder as a training set (shown in blue). The test error is estimated by averaging the five resulting MSE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

or linear discriminant analysis, or any of the methods discussed in later 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

k-fold CV

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, $\text{MSE}_1, \text{MSE}_2, \ldots, \text{MSE}_k$. The k-fold CV estimate is computed by averaging these values,

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

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

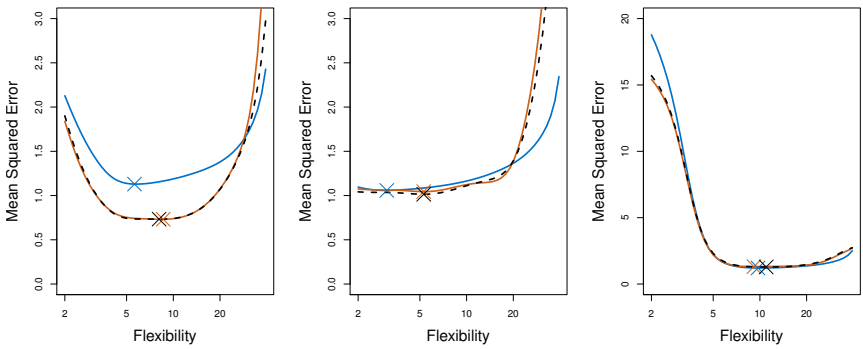


FIGURE 5.6. *True and estimated test MSE for the simulated data sets in Figures 2.9 (*left*), 2.10 (*center*), and 2.11 (*right*). The true test MSE is shown in blue, the LOOCV estimate is shown as a black dashed line, and the* 10*-fold CV estimate is shown in orange. The crosses indicate the minimum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

fitting procedures, and so performing LOOCV may pose computational problems, especially if n is extremely large. In contrast, performing 10-fold 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 approximately $(k-1)n/k$ 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

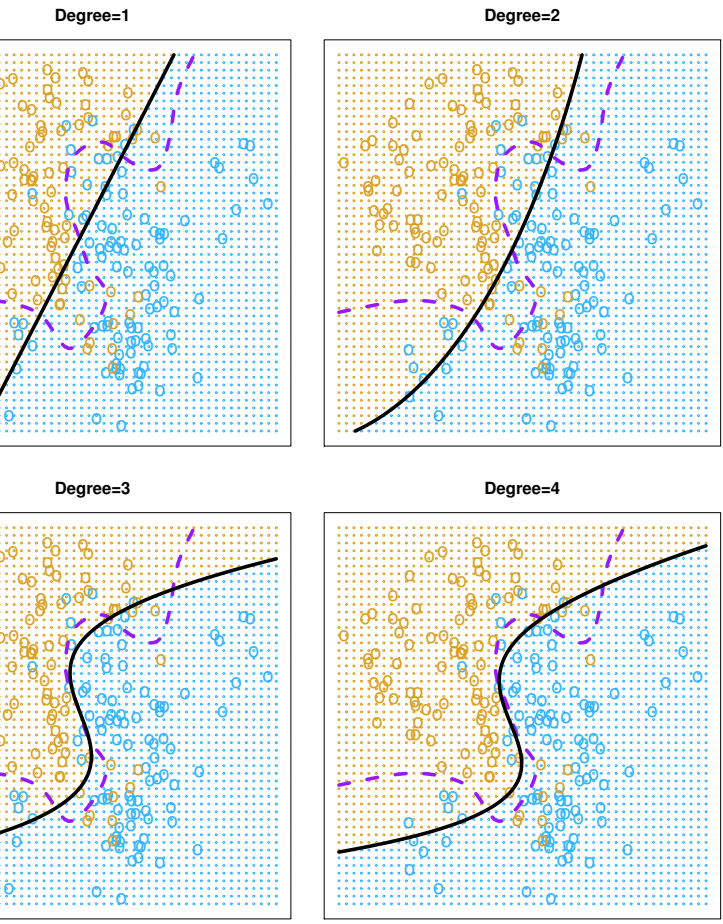
$$\mathrm{CV}_{(n)} = \frac{1}{n}\sum_{i=1}^{n} \mathrm{Err}_i, \tag{5.4}$$

where $\mathrm{Err}_i = I(y_i \neq \hat{y}_i)$. 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

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

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,



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

A much larger improvement is apparent in the bottom-left panel 5.7, in which we have fit a logistic regression model involving nomials of the predictors. Now the test error rate has decreased Going to a quartic polynomial (bottom-right) slightly increases ror.

ice, for real data, the Bayes decision boundary and the test er- re unknown. So how might we decide between the four logistic models displayed in Figure 5.7? We can use cross-validation in

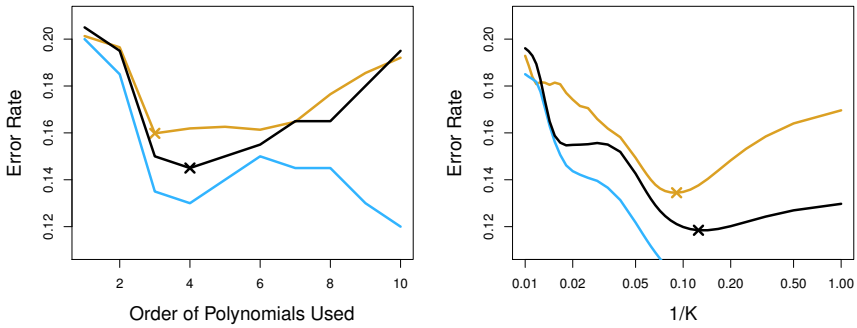


FIGURE 5.8. *Test error (brown), training error (blue), and* 10*-fold CV error (black) on the two-dimensional classification data displayed in Figure 5.7.* Left: *Logistic regression using polynomial functions of the predictors. The order of the polynomials used is displayed on the x-axis.* Right: *The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

order to make this decision. The left-hand panel of Figure 5.8 displays in 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.

5.2 The Bootstrap

The *bootstrap* is a widely applicable and extremely powerful statistical tool that can be used to quantify the uncertainty associated with a given estimator or statistical learning method. As a simple example, the bootstrap can be used to estimate the standard errors of the coefficients from a linear regression fit. In the specific case of linear regression, this is not particularly useful, since we saw in Chapter 3 that standard statistical software such as R outputs such standard errors automatically. However, the power of the bootstrap lies in the fact that it can be easily applied to a wide range of statistical learning methods, including some for which a measure of variability is otherwise difficult to obtain and is not automatically output by statistical software.

bootstrap

In this section we illustrate the bootstrap on a toy example in which we wish to determine the best investment allocation under a simple model. In Section 5.3 we explore the use of the bootstrap to assess the variability associated with the regression coefficients in a linear model fit.

Suppose that we wish to invest a fixed sum of money in two financial assets that yield returns of X and Y, respectively, where X and Y are random quantities. We will invest a fraction α of our money in X, and will invest the remaining $1-\alpha$ in Y. Since there is variability associated with the returns on these two assets, we wish to choose α to minimize the total risk, or variance, of our investment. In other words, we want to minimize $\text{Var}(\alpha X + (1-\alpha)Y)$. One can show that the value that minimizes the risk is given by

$$\alpha = \frac{\sigma_Y^2 - \sigma_{XY}}{\sigma_X^2 + \sigma_Y^2 - 2\sigma_{XY}}, \tag{5.6}$$

where $\sigma_X^2 = \text{Var}(X), \sigma_Y^2 = \text{Var}(Y)$, and $\sigma_{XY} = \text{Cov}(X, Y)$.

In reality, the quantities σ_X^2, σ_Y^2, and σ_{XY} are unknown. We can compute estimates for these quantities, $\hat{\sigma}_X^2$, $\hat{\sigma}_Y^2$, and $\hat{\sigma}_{XY}$, using a data set that contains past measurements for X and Y. We can then estimate the value of α that minimizes the variance of our investment using

$$\hat{\alpha} = \frac{\hat{\sigma}_Y^2 - \hat{\sigma}_{XY}}{\hat{\sigma}_X^2 + \hat{\sigma}_Y^2 - 2\hat{\sigma}_{XY}}. \tag{5.7}$$

Figure 5.9 illustrates this approach for estimating α on a simulated data set. In each panel, we simulated 100 pairs of returns for the investments X and Y. We used these returns to estimate σ_X^2, σ_Y^2, and σ_{XY}, which we then substituted into (5.7) in order to obtain estimates for α. The value of $\hat{\alpha}$ resulting from each simulated data set ranges from 0.532 to 0.657.

It is natural to wish to quantify the accuracy of our estimate of α. To estimate the standard deviation of $\hat{\alpha}$, we repeated the process of simulating 100 paired observations of X and Y, and estimating α using (5.7), 1,000 times. We thereby obtained 1,000 estimates for α, which we can call

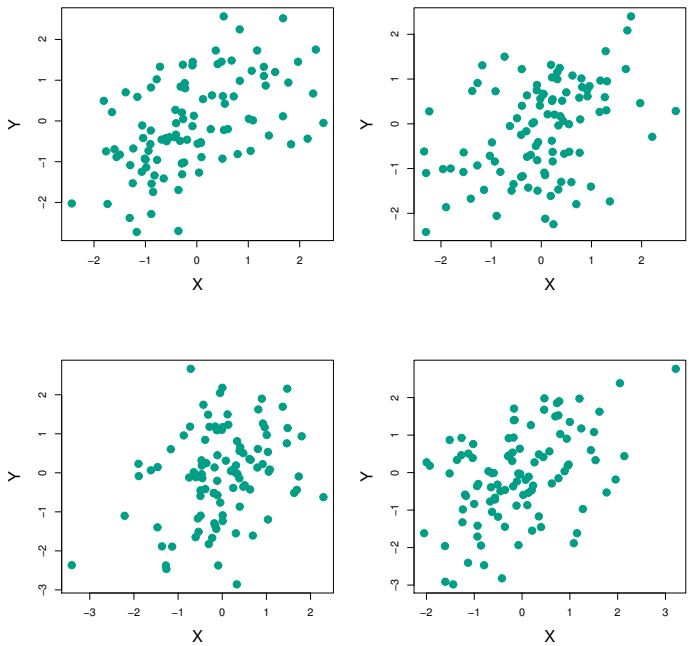


FIGURE 5.9. *Each panel displays* 100 *simulated returns for investments* X *and* Y. *From left to right and top to bottom, the resulting estimates for* α *are* 0.576, 0.532, 0.657, *and* 0.651.

$\hat{\alpha}_1, \hat{\alpha}_2, \ldots, \hat{\alpha}_{1,000}$. The left-hand panel of Figure 5.10 displays a histogram of the resulting estimates. For these simulations the parameters were set to $\sigma_X^2 = 1, \sigma_Y^2 = 1.25$, and $\sigma_{XY} = 0.5$, and so we know that the true value of α is 0.6. We indicated this value using a solid vertical line on the histogram. The mean over all 1,000 estimates for α is

$$\bar{\alpha} = \frac{1}{1000} \sum_{r=1}^{1000} \hat{\alpha}_r = 0.5996,$$

very close to $\alpha = 0.6$, and the standard deviation of the estimates is

$$\sqrt{\frac{1}{1000 - 1} \sum_{r=1}^{1000} (\hat{\alpha}_r - \bar{\alpha})^2} = 0.083.$$

This gives us a very good idea of the accuracy of $\hat{\alpha}$: $\mathrm{SE}(\hat{\alpha}) \approx 0.083$. So roughly speaking, for a random sample from the population, we would expect $\hat{\alpha}$ to differ from α by approximately 0.08, on average.

In practice, however, the procedure for estimating $\mathrm{SE}(\hat{\alpha})$ outlined above cannot be applied, because for real data we cannot generate new samples

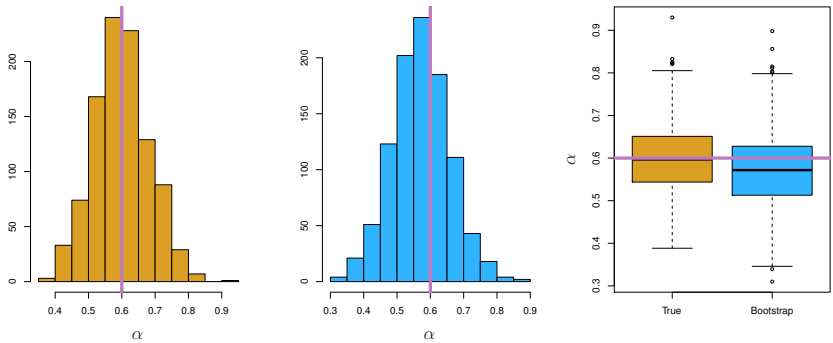


FIGURE 5.10. Left: *A histogram of the estimates of* α *obtained by generating 1,000 simulated data sets from the true population.* Center: *A histogram of the estimates of* α *obtained from 1,000 bootstrap samples from a single data set.* Right: *The estimates of* α *displayed in the left and center panels are shown as boxplots. In each panel, the pink line indicates the true value of* α.

from the original population. However, the bootstrap approach allows us to use a computer to emulate the process of obtaining new sample sets, so that we can estimate the variability of $\hat{\alpha}$ without generating additional samples. Rather than repeatedly obtaining independent data sets from the population, we instead obtain distinct data sets by repeatedly sampling observations *from the original data set.*

This approach is illustrated in Figure 5.11 on a simple data set, which we call Z, that contains only $n = 3$ observations. We randomly select n observations from the data set in order to produce a bootstrap data set, Z^{*1}. The sampling is performed *with replacement*, which means that the same observation can occur more than once in the bootstrap data set. In this example, Z^{*1} contains the third observation twice, the first observation once, and no instances of the second observation. Note that if an observation is contained in Z^{*1}, then both its X and Y values are included. We can use Z^{*1} to produce a new bootstrap estimate for α, which we call $\hat{\alpha}^{*1}$. This procedure is repeated B times for some large value of B, in order to produce B different bootstrap data sets, $Z^{*1}, Z^{*2}, \ldots, Z^{*B}$, and B corresponding α estimates, $\hat{\alpha}^{*1}, \hat{\alpha}^{*2}, \ldots, \hat{\alpha}^{*B}$. We can compute the standard error of these bootstrap estimates using the formula

with replacement

$$\mathrm{SE}_B(\hat{\alpha}) = \sqrt{\frac{1}{B-1}\sum_{r=1}^{B}\left(\hat{\alpha}^{*r} - \frac{1}{B}\sum_{r'=1}^{B}\hat{\alpha}^{*r'}\right)^2}. \tag{5.8}$$

This serves as an estimate of the standard error of $\hat{\alpha}$ estimated from the original data set.

The bootstrap approach is illustrated in the center panel of Figure 5.10, which displays a histogram of 1,000 bootstrap estimates of α, each com-

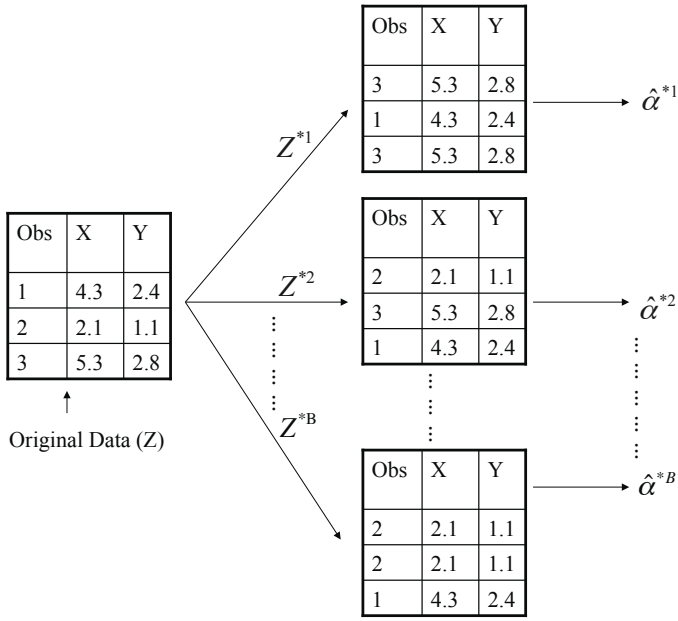


FIGURE 5.11. *A graphical illustration of the bootstrap approach on a small sample containing* $n = 3$ *observations. Each bootstrap data set contains* n *observations, sampled with replacement from the original data set. Each bootstrap data set is used to obtain an estimate of* α*.*

puted using a distinct bootstrap data set. This panel was constructed on the basis of a single data set, and hence could be created using real data. Note that the histogram looks very similar to the left-hand panel, which displays the idealized histogram of the estimates of α obtained by generating 1,000 simulated data sets from the true population. In particular the bootstrap estimate SE($\hat{\alpha}$) from (5.8) is 0.087, very close to the estimate of 0.083 obtained using 1,000 simulated data sets. The right-hand panel displays the information in the center and left panels in a different way, via boxplots of the estimates for α obtained by generating 1,000 simulated data sets from the true population and using the bootstrap approach. Again, the boxplots have similar spreads, indicating that the bootstrap approach can be used to effectively estimate the variability associated with $\hat{\alpha}$.

5.3 Lab: Cross-Validation and the Bootstrap

In this lab, we explore the resampling techniques covered in this chapter. Some of the commands in this lab may take a while to run on your computer.

5.3.1 The Validation Set Approach

We explore the use of the validation set approach in order to estimate the test error rates that result from fitting various linear models on the `Auto` data set.

Before we begin, we use the `set.seed()` function in order to set a *seed* for `R`'s random number generator, so that the reader of this book will obtain precisely the same results as those shown below. It is generally a good idea to set a random seed when performing an analysis such as cross-validation that contains an element of randomness, so that the results obtained can be reproduced precisely at a later time.

seed

We begin by using the `sample()` function to split the set of observations into two halves, by selecting a random subset of 196 observations out of the original 392 observations. We refer to these observations as the training set.

sample()

```
> library(ISLR2)
> set.seed(1)
> train <- sample(392, 196)
```

(Here we use a shortcut in the sample command; see `?sample` for details.) We then use the `subset` option in `lm()` to fit a linear regression using only the observations corresponding to the training set.

```
> lm.fit <- lm(mpg ~ horsepower, data = Auto, subset = train)
```

We now use the `predict()` function to estimate the response for all 392 observations, and we use the `mean()` function to calculate the MSE of the 196 observations in the validation set. Note that the `-train` index below selects only the observations that are not in the training set.

```
> attach(Auto)
> mean((mpg - predict(lm.fit, Auto))[-train]^2)
[1] 23.27
```

Therefore, the estimated test MSE for the linear regression fit is 23.27. We can use the `poly()` function to estimate the test error for the quadratic and cubic regressions.

```
> lm.fit2 <- lm(mpg ~ poly(horsepower, 2), data = Auto,
    subset = train)
> mean((mpg - predict(lm.fit2, Auto))[-train]^2)
[1] 18.72
> lm.fit3 <- lm(mpg ~ poly(horsepower, 3), data = Auto,
    subset = train)
> mean((mpg - predict(lm.fit3, Auto))[-train]^2)
[1] 18.79
```

These error rates are 18.72 and 18.79, respectively. If we choose a different training set instead, then we will obtain somewhat different errors on the validation set.

```
> set.seed(2)
> train <- sample(392, 196)
> lm.fit <- lm(mpg ~ horsepower, subset = train)
> mean((mpg - predict(lm.fit, Auto))[-train]^2)
[1] 25.73
> lm.fit2 <- lm(mpg ~ poly(horsepower, 2), data = Auto,
    subset = train)
> mean((mpg - predict(lm.fit2, Auto))[-train]^2)
[1] 20.43
> lm.fit3 <- lm(mpg ~ poly(horsepower, 3), data = Auto,
    subset = train)
> mean((mpg - predict(lm.fit3, Auto))[-train]^2)
[1] 20.39
```

Using this split of the observations into a training set and a validation set, we find that the validation set error rates for the models with linear, quadratic, and cubic terms are 25.73, 20.43, and 20.39, respectively.

These results are consistent with our previous findings: a model that predicts `mpg` using a quadratic function of `horsepower` performs better than a model that involves only a linear function of `horsepower`, and there is little evidence in favor of a model that uses a cubic function of `horsepower`.

5.3.2 Leave-One-Out Cross-Validation

The LOOCV estimate can be automatically computed for any generalized linear model using the `glm()` and `cv.glm()` functions. In the lab for Chapter 4, we used the `glm()` function to perform logistic regression by passing in the `family = "binomial"` argument. But if we use `glm()` to fit a model without passing in the `family` argument, then it performs linear regression, just like the `lm()` function. So for instance,

`cv.glm()`

```
> glm.fit <- glm(mpg ~ horsepower, data = Auto)
> coef(glm.fit)
(Intercept)  horsepower
     39.936      -0.158
```

and

```
> lm.fit <- lm(mpg ~ horsepower, data = Auto)
> coef(lm.fit)
(Intercept)  horsepower
     39.936      -0.158
```

yield identical linear regression models. In this lab, we will perform linear regression using the `glm()` function rather than the `lm()` function because the former can be used together with `cv.glm()`. The `cv.glm()` function is part of the `boot` library.

```
> library(boot)
> glm.fit <- glm(mpg ~ horsepower, data = Auto)
> cv.err <- cv.glm(Auto, glm.fit)
> cv.err$delta
```

```
    1     1
24.23 24.23
```

The `cv.glm()` function produces a list with several components. The two numbers in the `delta` vector contain the cross-validation results. In this case the numbers are identical (up to two decimal places) and correspond to the LOOCV statistic given in (5.1). Below, we discuss a situation in which the two numbers differ. Our cross-validation estimate for the test error is approximately 24.23.

We can repeat this procedure for increasingly complex polynomial fits. To automate the process, we use the `for()` function to initiate a *for loop* which iteratively fits polynomial regressions for polynomials of order $i = 1$ to $i = 10$, computes the associated cross-validation error, and stores it in the ith element of the vector `cv.error`. We begin by initializing the vector.

`for()`
for loop

```
> cv.error <- rep(0, 10)
> for (i in 1:10) {
+   glm.fit <- glm(mpg ~ poly(horsepower, i), data = Auto)
+   cv.error[i] <- cv.glm(Auto, glm.fit)$delta[1]
+ }
> cv.error
[1] 24.23 19.25 19.33 19.42 19.03 18.98 18.83 18.96 19.07 19.49
```

As in Figure 5.4, we see a sharp drop in the estimated test MSE between the linear and quadratic fits, but then no clear improvement from using higher-order polynomials.

5.3.3 *k-Fold Cross-Validation*

The `cv.glm()` function can also be used to implement k-fold CV. Below we use $k = 10$, a common choice for k, on the `Auto` data set. We once again set a random seed and initialize a vector in which we will store the CV errors corresponding to the polynomial fits of orders one to ten.

```
> set.seed(17)
> cv.error.10 <- rep(0, 10)
> for (i in 1:10) {
+   glm.fit <- glm(mpg ~ poly(horsepower, i), data = Auto)
+   cv.error.10[i] <- cv.glm(Auto, glm.fit, K = 10)$delta[1]
+ }
> cv.error.10
[1] 24.27 19.27 19.35 19.29 19.03 18.90 19.12 19.15 18.87 20.96
```

Notice that the computation time is shorter than that of LOOCV. (In principle, the computation time for LOOCV for a least squares linear model should be faster than for k-fold CV, due to the availability of the formula (5.2) for LOOCV; however, unfortunately the `cv.glm()` function does not make use of this formula.) We still see little evidence that using cubic or higher-order polynomial terms leads to lower test error than simply using a quadratic fit.

We saw in Section 5.3.2 that the two numbers associated with `delta` are essentially the same when LOOCV is performed. When we instead perform k-fold CV, then the two numbers associated with `delta` differ slightly. The first is the standard k-fold CV estimate, as in (5.3). The second is a bias-corrected version. On this data set, the two estimates are very similar to each other.

5.3.4 The Bootstrap

We illustrate the use of the bootstrap in the simple example of Section 5.2, as well as on an example involving estimating the accuracy of the linear regression model on the `Auto` data set.

Estimating the Accuracy of a Statistic of Interest

One of the great advantages of the bootstrap approach is that it can be applied in almost all situations. No complicated mathematical calculations are required. Performing a bootstrap analysis in `R` entails only two steps. First, we must create a function that computes the statistic of interest. Second, we use the `boot()` function, which is part of the `boot` library, to perform the bootstrap by repeatedly sampling observations from the data set with replacement.

`boot()`

The `Portfolio` data set in the `ISLR2` package is simulated data of 100 pairs of returns, generated in the fashion described in Section 5.2. To illustrate the use of the bootstrap on this data, we must first create a function, `alpha.fn()`, which takes as input the (X, Y) data as well as a vector indicating which observations should be used to estimate α. The function then outputs the estimate for α based on the selected observations.

```
> alpha.fn <- function(data, index) {
+   X <- data$X[index]
+   Y <- data$Y[index]
+   (var(Y) - cov(X, Y)) / (var(X) + var(Y) - 2 * cov(X, Y))
+ }
```

This function *returns*, or outputs, an estimate for α based on applying (5.7) to the observations indexed by the argument `index`. For instance, the following command tells `R` to estimate α using all 100 observations.

```
> alpha.fn(Portfolio, 1:100)
[1] 0.576
```

The next command uses the `sample()` function to randomly select 100 observations from the range 1 to 100, with replacement. This is equivalent to constructing a new bootstrap data set and recomputing $\hat{\alpha}$ based on the new data set.

```
> set.seed(7)
> alpha.fn(Portfolio, sample(100, 100, replace = T))
[1] 0.539
```

We can implement a bootstrap analysis by performing this command many times, recording all of the corresponding estimates for α, and computing the resulting standard deviation. However, the `boot()` function automates this approach. Below we produce $R = 1,000$ bootstrap estimates for α.

`boot()`

```
> boot(Portfolio, alpha.fn, R = 1000)

ORDINARY NONPARAMETRIC BOOTSTRAP

Call:
boot(data = Portfolio, statistic = alpha.fn, R = 1000)

Bootstrap Statistics :
     original      bias      std. error
t1*  0.5758       0.001      0.0897
```

The final output shows that using the original data, $\hat{\alpha} = 0.5758$, and that the bootstrap estimate for $\text{SE}(\hat{\alpha})$ is 0.0897.

Estimating the Accuracy of a Linear Regression Model

The bootstrap approach can be used to assess the variability of the coefficient estimates and predictions from a statistical learning method. Here we use the bootstrap approach in order to assess the variability of the estimates for β_0 and β_1, the intercept and slope terms for the linear regression model that uses `horsepower` to predict `mpg` in the `Auto` data set. We will compare the estimates obtained using the bootstrap to those obtained using the formulas for $\text{SE}(\hat{\beta}_0)$ and $\text{SE}(\hat{\beta}_1)$ described in Section 3.1.2.

We first create a simple function, `boot.fn()`, which takes in the `Auto` data set as well as a set of indices for the observations, and returns the intercept and slope estimates for the linear regression model. We then apply this function to the full set of 392 observations in order to compute the estimates of β_0 and β_1 on the entire data set using the usual linear regression coefficient estimate formulas from Chapter 3. Note that we do not need the `{` and `}` at the beginning and end of the function because it is only one line long.

```
> boot.fn <- function(data, index)
+   coef(lm(mpg ~ horsepower, data = data, subset = index))
> boot.fn(Auto, 1:392)
(Intercept) horsepower
   39.936  -0.158
```

The `boot.fn()` function can also be used in order to create bootstrap estimates for the intercept and slope terms by randomly sampling from among the observations with replacement. Here we give two examples.

```
> set.seed(1)
> boot.fn(Auto, sample(392, 392, replace = T))
(Intercept) horsepower
  40.341     -0.164
```

```
> boot.fn(Auto, sample(392, 392, replace = T))
(Intercept) horsepower
  40.119      -0.158
```

Next, we use the `boot()` function to compute the standard errors of 1,000 bootstrap estimates for the intercept and slope terms.

```
> boot(Auto, boot.fn, 1000)

ORDINARY NONPARAMETRIC BOOTSTRAP

Call:
boot(data = Auto, statistic = boot.fn, R = 1000)

Bootstrap Statistics :
    original    bias    std. error
t1*  39.936   0.0545     0.8413
t2*  -0.158  -0.0006     0.0073
```

This indicates that the bootstrap estimate for $\mathrm{SE}(\hat{\beta}_0)$ is 0.84, and that the bootstrap estimate for $\mathrm{SE}(\hat{\beta}_1)$ is 0.0073. As discussed in Section 3.1.2, standard formulas can be used to compute the standard errors for the regression coefficients in a linear model. These can be obtained using the `summary()` function.

```
> summary(lm(mpg ~ horsepower, data = Auto))$coef
             Estimate Std. Error t value  Pr(>|t|)
(Intercept)   39.936    0.71750    55.7 1.22e-187
horsepower    -0.158    0.00645   -24.5  7.03e-81
```

The standard error estimates for $\hat{\beta}_0$ and $\hat{\beta}_1$ obtained using the formulas from Section 3.1.2 are 0.717 for the intercept and 0.0064 for the slope. Interestingly, these are somewhat different from the estimates obtained using the bootstrap. Does this indicate a problem with the bootstrap? In fact, it suggests the opposite. Recall that the standard formulas given in Equation 3.8 on page 66 rely on certain assumptions. For example, they depend on the unknown parameter σ^2, the noise variance. We then estimate σ^2 using the RSS. Now although the formulas for the standard errors do not rely on the linear model being correct, the estimate for σ^2 does. We see in Figure 3.8 on page 92 that there is a non-linear relationship in the data, and so the residuals from a linear fit will be inflated, and so will $\hat{\sigma}^2$. Secondly, the standard formulas assume (somewhat unrealistically) that the x_i are fixed, and all the variability comes from the variation in the errors ϵ_i. The bootstrap approach does not rely on any of these assumptions, and so it is likely giving a more accurate estimate of the standard errors of $\hat{\beta}_0$ and $\hat{\beta}_1$ than is the `summary()` function.

Below we compute the bootstrap standard error estimates and the standard linear regression estimates that result from fitting the quadratic model to the data. Since this model provides a good fit to the data (Figure 3.8),

there is now a better correspondence between the bootstrap estimates and the standard estimates of $\text{SE}(\hat{\beta}_0)$, $\text{SE}(\hat{\beta}_1)$ and $\text{SE}(\hat{\beta}_2)$.

```
> boot.fn <- function(data, index)
+   coef(
      lm(mpg ~ horsepower + I(horsepower^2),
        data = data, subset = index)
    )
> set.seed(1)
> boot(Auto, boot.fn, 1000)

ORDINARY NONPARAMETRIC BOOTSTRAP

Call:
boot(data = Auto, statistic = boot.fn, R = 1000)

Bootstrap Statistics :
     original    bias    std. error
t1*  56.9001   3.51e-02   2.0300
t2*  -0.4661  -7.08e-04   0.0324
t3*   0.0012   2.84e-06   0.0001

> summary(
    lm(mpg ~ horsepower + I(horsepower^2), data = Auto)
  )$coef
                Estimate Std. Error t value Pr(>|t|)
(Intercept)      56.9001    1.8004      32  1.7e-109
horsepower       -0.4662    0.0311     -15  2.3e-40
I(horsepower^2)   0.0012    0.0001      10  2.2e-21
```

5.4 Exercises

Conceptual

1. Using basic statistical properties of the variance, as well as single-variable calculus, derive (5.6). In other words, prove that α given by (5.6) does indeed minimize $\text{Var}(\alpha X + (1-\alpha)Y)$.

2. We will now derive the probability that a given observation is part of a bootstrap sample. Suppose that we obtain a bootstrap sample from a set of n observations.

   (a) What is the probability that the first bootstrap observation is *not* the jth observation from the original sample? Justify your answer.

   (b) What is the probability that the second bootstrap observation is *not* the jth observation from the original sample?

   (c) Argue that the probability that the jth observation is *not* in the bootstrap sample is $(1-1/n)^n$.

(d) When $n = 5$, what is the probability that the jth observation is in the bootstrap sample?

(e) When $n = 100$, what is the probability that the jth observation is in the bootstrap sample?

(f) When $n = 10,000$, what is the probability that the jth observation is in the bootstrap sample?

(g) Create a plot that displays, for each integer value of n from 1 to $100,000$, the probability that the jth observation is in the bootstrap sample. Comment on what you observe.

(h) We will now investigate numerically the probability that a bootstrap sample of size $n = 100$ contains the jth observation. Here $j = 4$. We repeatedly create bootstrap samples, and each time we record whether or not the fourth observation is contained in the bootstrap sample.

```
> store <- rep(NA, 10000)
> for(i in 1:10000){
    store[i] <- sum(sample(1:100, rep=TRUE) == 4) > 0
}
> mean(store)
```

Comment on the results obtained.

3. We now review k-fold cross-validation.

(a) Explain how k-fold cross-validation is implemented.

(b) What are the advantages and disadvantages of k-fold cross-validation relative to:

i. The validation set approach?

ii. LOOCV?

4. Suppose that we use some statistical learning method to make a prediction for the response Y for a particular value of the predictor X. Carefully describe how we might estimate the standard deviation of our prediction.

Applied

5. In Chapter 4, we used logistic regression to predict the probability of `default` using `income` and `balance` on the `Default` data set. We will now estimate the test error of this logistic regression model using the validation set approach. Do not forget to set a random seed before beginning your analysis.

(a) Fit a logistic regression model that uses `income` and `balance` to predict `default`.

(b) Using the validation set approach, estimate the test error of this model. In order to do this, you must perform the following steps:
   i. Split the sample set into a training set and a validation set.
   ii. Fit a multiple logistic regression model using only the training observations.
   iii. Obtain a prediction of default status for each individual in the validation set by computing the posterior probability of default for that individual, and classifying the individual to the `default` category if the posterior probability is greater than 0.5.
   iv. Compute the validation set error, which is the fraction of the observations in the validation set that are misclassified.

(c) Repeat the process in (b) three times, using three different splits of the observations into a training set and a validation set. Comment on the results obtained.

(d) Now consider a logistic regression model that predicts the probability of `default` using `income`, `balance`, and a dummy variable for `student`. Estimate the test error for this model using the validation set approach. Comment on whether or not including a dummy variable for `student` leads to a reduction in the test error rate.

6. We continue to consider the use of a logistic regression model to predict the probability of `default` using `income` and `balance` on the `Default` data set. In particular, we will now compute estimates for the standard errors of the `income` and `balance` logistic regression coefficients in two different ways: (1) using the bootstrap, and (2) using the standard formula for computing the standard errors in the `glm()` function. Do not forget to set a random seed before beginning your analysis.

(a) Using the `summary()` and `glm()` functions, determine the estimated standard errors for the coefficients associated with `income` and `balance` in a multiple logistic regression model that uses both predictors.

(b) Write a function, `boot.fn()`, that takes as input the `Default` data set as well as an index of the observations, and that outputs the coefficient estimates for `income` and `balance` in the multiple logistic regression model.

(c) Use the `boot()` function together with your `boot.fn()` function to estimate the standard errors of the logistic regression coefficients for `income` and `balance`.

(d) Comment on the estimated standard errors obtained using the `glm()` function and using your bootstrap function.

7. In Sections 5.3.2 and 5.3.3, we saw that the `cv.glm()` function can be used in order to compute the LOOCV test error estimate. Alternatively, one could compute those quantities using just the `glm()` and `predict.glm()` functions, and a for loop. You will now take this approach in order to compute the LOOCV error for a simple logistic regression model on the `Weekly` data set. Recall that in the context of classification problems, the LOOCV error is given in (5.4).

   (a) Fit a logistic regression model that predicts `Direction` using `Lag1` and `Lag2`.

   (b) Fit a logistic regression model that predicts `Direction` using `Lag1` and `Lag2` *using all but the first observation.*

   (c) Use the model from (b) to predict the direction of the first observation. You can do this by predicting that the first observation will go up if $P(\texttt{Direction = "Up"}|\texttt{Lag1}, \texttt{Lag2}) > 0.5$. Was this observation correctly classified?

   (d) Write a for loop from $i = 1$ to $i = n$, where n is the number of observations in the data set, that performs each of the following steps:

      i. Fit a logistic regression model using all but the ith observation to predict `Direction` using `Lag1` and `Lag2`.

      ii. Compute the posterior probability of the market moving up for the ith observation.

      iii. Use the posterior probability for the ith observation in order to predict whether or not the market moves up.

      iv. Determine whether or not an error was made in predicting the direction for the ith observation. If an error was made, then indicate this as a 1, and otherwise indicate it as a 0.

   (e) Take the average of the n numbers obtained in (d)iv in order to obtain the LOOCV estimate for the test error. Comment on the results.

8. We will now perform cross-validation on a simulated data set.

   (a) Generate a simulated data set as follows:

```
> set.seed(1)
> x <- rnorm(100)
> y <- x - 2 * x^2 + rnorm(100)
```

   In this data set, what is n and what is p? Write out the model used to generate the data in equation form.

   (b) Create a scatterplot of X against Y. Comment on what you find.

   (c) Set a random seed, and then compute the LOOCV errors that result from fitting the following four models using least squares:

i. $Y = \beta_0 + \beta_1 X + \epsilon$
ii. $Y = \beta_0 + \beta_1 X + \beta_2 X^2 + \epsilon$
iii. $Y = \beta_0 + \beta_1 X + \beta_2 X^2 + \beta_3 X^3 + \epsilon$
iv. $Y = \beta_0 + \beta_1 X + \beta_2 X^2 + \beta_3 X^3 + \beta_4 X^4 + \epsilon$.

Note you may find it helpful to use the `data.frame()` function to create a single data set containing both X and Y.

(d) Repeat (c) using another random seed, and report your results. Are your results the same as what you got in (c)? Why?

(e) Which of the models in (c) had the smallest LOOCV error? Is this what you expected? Explain your answer.

(f) Comment on the statistical significance of the coefficient estimates that results from fitting each of the models in (c) using least squares. Do these results agree with the conclusions drawn based on the cross-validation results?

9. We will now consider the `Boston` housing data set, from the `ISLR2` library.

(a) Based on this data set, provide an estimate for the population mean of `medv`. Call this estimate $\hat{\mu}$.

(b) Provide an estimate of the standard error of $\hat{\mu}$. Interpret this result.
Hint: We can compute the standard error of the sample mean by dividing the sample standard deviation by the square root of the number of observations.

(c) Now estimate the standard error of $\hat{\mu}$ using the bootstrap. How does this compare to your answer from (b)?

(d) Based on your bootstrap estimate from (c), provide a 95 % confidence interval for the mean of `medv`. Compare it to the results obtained using `t.test(Boston$medv)`.
Hint: You can approximate a 95 % confidence interval using the formula $[\hat{\mu} - 2\text{SE}(\hat{\mu}), \hat{\mu} + 2\text{SE}(\hat{\mu})]$.

(e) Based on this data set, provide an estimate, $\hat{\mu}_{med}$, for the median value of `medv` in the population.

(f) We now would like to estimate the standard error of $\hat{\mu}_{med}$. Unfortunately, there is no simple formula for computing the standard error of the median. Instead, estimate the standard error of the median using the bootstrap. Comment on your findings.

(g) Based on this data set, provide an estimate for the tenth percentile of `medv` in Boston census tracts. Call this quantity $\hat{\mu}_{0.1}$. (You can use the `quantile()` function.)

(h) Use the bootstrap to estimate the standard error of $\hat{\mu}_{0.1}$. Comment on your findings.

6

Linear Model Selection and Regularization

In the regression setting, the standard linear model

$$Y = \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p + \epsilon \tag{6.1}$$

is commonly used to describe the relationship between a response Y and a set of variables $X_1, X_2, \ldots, X_p$. We have seen in Chapter 3 that one typically fits this model using least squares.

In the chapters that follow, we consider some approaches for extending the linear model framework. In Chapter 7 we generalize (6.1) in order to accommodate non-linear, but still additive, relationships, while in Chapters 8 and 10 we consider even more general non-linear models. However, the linear model has distinct advantages in terms of inference and, on real-world problems, is often surprisingly competitive in relation to non-linear methods. Hence, before moving to the non-linear world, we discuss in this chapter some ways in which the simple linear model can be improved, by replacing plain least squares fitting with some alternative fitting procedures.

Why might we want to use another fitting procedure instead of least squares? As we will see, alternative fitting procedures can yield better *prediction accuracy* and *model interpretability*.

- *Prediction Accuracy*: Provided that the true relationship between the response and the predictors is approximately linear, the least squares estimates will have low bias. If $n \gg p$—that is, if n, the number of observations, is much larger than p, the number of variables—then the least squares estimates tend to also have low variance, and hence will perform well on test observations. However, if n is not much larger

than p, then there can be a lot of variability in the least squares fit, resulting in overfitting and consequently poor predictions on future observations not used in model training. And if $p > n$, then there is no longer a unique least squares coefficient estimate: there are infinitely many solutions. Each of these least squares solutions gives zero error on the training data, but typically very poor test set performance due to extremely high variance.[1] By *constraining* or *shrinking* the estimated coefficients, we can often substantially reduce the variance at the cost of a negligible increase in bias. This can lead to substantial improvements in the accuracy with which we can predict the response for observations not used in model training.

- *Model Interpretability*: It is often the case that some or many of the variables used in a multiple regression model are in fact not associated with the response. Including such *irrelevant* variables leads to unnecessary complexity in the resulting model. By removing these variables—that is, by setting the corresponding coefficient estimates to zero—we can obtain a model that is more easily interpreted. Now least squares is extremely unlikely to yield any coefficient estimates that are exactly zero. In this chapter, we see some approaches for automatically performing *feature selection* or *variable selection*—that is, for excluding irrelevant variables from a multiple regression model.

feature selection
variable selection

There are many alternatives, both classical and modern, to using least squares to fit (6.1). In this chapter, we discuss three important classes of methods.

- *Subset Selection.* This approach involves identifying a subset of the p predictors that we believe to be related to the response. We then fit a model using least squares on the reduced set of variables.

- *Shrinkage.* This approach involves fitting a model involving all p predictors. However, the estimated coefficients are shrunken towards zero relative to the least squares estimates. This shrinkage (also known as *regularization*) has the effect of reducing variance. Depending on what type of shrinkage is performed, some of the coefficients may be estimated to be exactly zero. Hence, shrinkage methods can also perform variable selection.

- *Dimension Reduction.* This approach involves *projecting* the p predictors into an M-dimensional subspace, where $M < p$. This is achieved by computing M different *linear combinations*, or *projections*, of the variables. Then these M projections are used as predictors to fit a linear regression model by least squares.

[1] When $p \gg n$, the least squares solution that has the smallest sum of squared coefficients can sometimes perform quite well. See Section 10.8 for a more detailed discussion.

In the following sections we describe each of these approaches in greater detail, along with their advantages and disadvantages. Although this chapter describes extensions and modifications to the linear model for regression seen in Chapter 3, the same concepts apply to other methods, such as the classification models seen in Chapter 4.

6.1 Subset Selection

In this section we consider some methods for selecting subsets of predictors. These include best subset and stepwise model selection procedures.

6.1.1 Best Subset Selection

best subset selection

To perform *best subset selection*, we fit a separate least squares regression for each possible combination of the p predictors. That is, we fit all p models that contain exactly one predictor, all $\binom{p}{2} = p(p-1)/2$ models that contain exactly two predictors, and so forth. We then look at all of the resulting models, with the goal of identifying the one that is *best*.

The problem of selecting the *best model* from among the 2^p possibilities considered by best subset selection is not trivial. This is usually broken up into two stages, as described in Algorithm 6.1.

Algorithm 6.1 *Best subset selection*

1. Let $\mathcal{M}_0$ denote the *null model*, which contains no predictors. This model simply predicts the sample mean for each observation.
2. For $k = 1, 2, \ldots p$:
   (a) Fit all $\binom{p}{k}$ models that contain exactly k predictors.
   (b) Pick the best among these $\binom{p}{k}$ models, and call it $\mathcal{M}_k$. Here *best* is defined as having the smallest RSS, or equivalently largest R^2.
3. Select a single best model from among $\mathcal{M}_0, \ldots, \mathcal{M}_p$ using using the prediction error on a validation set, C_p (AIC), BIC, or adjusted R^2. Or use the cross-validation method.

In Algorithm 6.1, Step 2 identifies the best model (on the training data) for each subset size, in order to reduce the problem from one of 2^p possible models to one of $p + 1$ possible models. In Figure 6.1, these models form the lower frontier depicted in red.

Now in order to select a single best model, we must simply choose among these $p + 1$ options. This task must be performed with care, because the

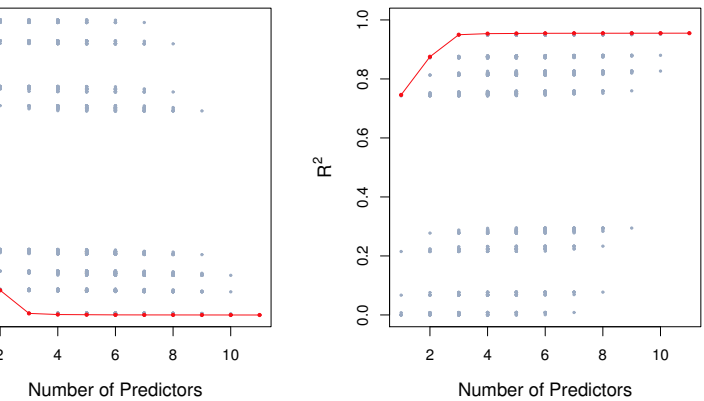
RSS of these $p + 1$ models decreases monotonically, and the R^2 increases monotonically, as the number of features included in the models increases. Therefore, if we use these statistics to select the best model, then we will always end up with a model involving all of the variables. The problem is that a low RSS or a high R^2 indicates a model with a low *training* error, whereas we wish to choose a model that has a low *test* error. (As shown in Chapter 2 in Figures 2.9–2.11, training error tends to be quite a bit smaller than test error, and a low training error by no means guarantees a low test error.) Therefore, in Step 3, we use the error on a validation set, C_p, BIC, or adjusted R^2 in order to select among $\mathcal{M}_0, \mathcal{M}_1, \ldots, \mathcal{M}_p$. If cross-validation is used to select the best model, then Step 2 is repeated on each training fold, and the validation errors are averaged to select the best value of k. Then the model $\mathcal{M}_k$ fit on the full training set is delivered for the chosen k. These approaches are discussed in Section 6.1.3.

An application of best subset selection is shown in Figure 6.1. Each plotted point corresponds to a least squares regression model fit using a different subset of the 10 predictors in the `Credit` data set, discussed in Chapter 3. Here the variable `region` is a three-level qualitative variable, and so is represented by two dummy variables, which are selected separately in this case. Hence, there are a total of 11 possible variables which can be included in the model. We have plotted the RSS and R^2 statistics for each model, as a function of the number of variables. The red curves connect the best models for each model size, according to RSS or R^2. The figure shows that, as expected, these quantities improve as the number of variables increases; however, from the three-variable model on, there is little improvement in RSS and R^2 as a result of including additional predictors.

Although we have presented best subset selection here for least squares regression, the same ideas apply to other types of models, such as logistic regression. In the case of logistic regression, instead of ordering models by RSS in Step 2 of Algorithm 6.1, we instead use the *deviance*, a measure that plays the role of RSS for a broader class of models. The deviance is negative two times the maximized log-likelihood; the smaller the deviance, the better the fit.

deviance

While best subset selection is a simple and conceptually appealing approach, it suffers from computational limitations. The number of possible models that must be considered grows rapidly as p increases. In general, there are 2^p models that involve subsets of p predictors. So if $p = 10$, then there are approximately 1,000 possible models to be considered, and if $p = 20$, then there are over one million possibilities! Consequently, best subset selection becomes computationally infeasible for values of p greater than around 40, even with extremely fast modern computers. There are computational shortcuts—so called branch-and-bound techniques—for eliminating some choices, but these have their limitations as p gets large. They also only work for least squares linear regression. We present computationally efficient alternatives to best subset selection next.



6.1. *For each possible model containing a subset of the ten predictors* `it` *data set, the RSS and* R^2 *are displayed. The red frontier tracks the for a given number of predictors, according to RSS and* R^2*. Though contains only ten predictors, the x-axis ranges from* 1 *to* 11*, since one bles is categorical and takes on three values, leading to the creation of variables.*

tepwise Selection

utational reasons, best subset selection cannot be applied with *p*. Best subset selection may also suffer from statistical problems arge. The larger the search space, the higher the chance of finding at look good on the training data, even though they might not predictive power on future data. Thus an enormous search space o overfitting and high variance of the coefficient estimates.
n of these reasons, *stepwise* methods, which explore a far more set of models, are attractive alternatives to best subset selection.

tepwise Selection

epwise selection is a computationally efficient alternative to best ection. While the best subset selection procedure considers all e models containing subsets of the p predictors, forward step- ders a much smaller set of models. Forward stepwise selection h a model containing no predictors, and then adds predictors del, one-at-a-time, until all of the predictors are in the model. lar, at each step the variable that gives the greatest *additional* ent to the fit is added to the model. More formally, the forward election procedure is given in Algorithm 6.2.

forward stepwise selection

Algorithm 6.2 *Forward stepwise selection*

1. Let $\mathcal{M}_0$ denote the *null* model, which contains no predictors.
2. For $k = 0, \ldots, p-1$:
   (a) Consider all $p-k$ models that augment the predictors in $\mathcal{M}_k$ with one additional predictor.
   (b) Choose the *best* among these $p-k$ models, and call it $\mathcal{M}_{k+1}$. Here *best* is defined as having smallest RSS or highest R^2.
3. Select a single best model from among $\mathcal{M}_0, \ldots, \mathcal{M}_p$ using the prediction error on a validation set, C_p (AIC), BIC, or adjusted R^2. Or use the cross-validation method.

Unlike best subset selection, which involved fitting 2^p models, forward stepwise selection involves fitting one null model, along with $p-k$ models in the kth iteration, for $k = 0, \ldots, p-1$. This amounts to a total of $1 + \sum_{k=0}^{p-1}(p-k) = 1+p(p+1)/2$ models. This is a substantial difference: when $p = 20$, best subset selection requires fitting 1,048,576 models, whereas forward stepwise selection requires fitting only 211 models.[2]

In Step 2(b) of Algorithm 6.2, we must identify the *best* model from among those $p-k$ that augment $\mathcal{M}_k$ with one additional predictor. We can do this by simply choosing the model with the lowest RSS or the highest R^2. However, in Step 3, we must identify the best model among a set of models with different numbers of variables. This is more challenging, and is discussed in Section 6.1.3.

Forward stepwise selection's computational advantage over best subset selection is clear. Though forward stepwise tends to do well in practice, it is not guaranteed to find the best possible model out of all 2^p models containing subsets of the p predictors. For instance, suppose that in a given data set with $p = 3$ predictors, the best possible one-variable model contains X_1, and the best possible two-variable model instead contains X_2 and X_3. Then forward stepwise selection will fail to select the best possible two-variable model, because $\mathcal{M}_1$ will contain X_1, so $\mathcal{M}_2$ must also contain X_1 together with one additional variable.

Table 6.1, which shows the first four selected models for best subset and forward stepwise selection on the `Credit` data set, illustrates this phenomenon. Both best subset selection and forward stepwise selection choose `rating` for the best one-variable model and then include `income` and `student` for the two- and three-variable models. However, best subset selection replaces `rating` by `cards` in the four-variable model, while forward stepwise

[2]Though forward stepwise selection considers $p(p+1)/2+1$ models, it performs a *guided* search over model space, and so the *effective* model space considered contains substantially more than $p(p+1)/2+1$ models.

# Variables	Best subset	Forward stepwise
One	`rating`	`rating`
Two	`rating`, `income`	`rating`, `income`
Three	`rating`, `income`, `student`	`rating`, `income`, `student`
Four	`cards`, `income` `student`, `limit`	`rating`, `income`, `student`, `limit`

TABLE 6.1. *The first four selected models for best subset selection and forward stepwise selection on the* `Credit` *data set. The first three models are identical but the fourth models differ.*

selection must maintain `rating` in its four-variable model. In this example, Figure 6.1 indicates that there is not much difference between the three- and four-variable models in terms of RSS, so either of the four-variable models will likely be adequate.

Forward stepwise selection can be applied even in the high-dimensional setting where $n < p$; however, in this case, it is possible to construct submodels $\mathcal{M}_0, \ldots, \mathcal{M}_{n-1}$ only, since each submodel is fit using least squares, which will not yield a unique solution if $p \geq n$.

Backward Stepwise Selection

backward stepwise selection

Like forward stepwise selection, *backward stepwise selection* provides an efficient alternative to best subset selection. However, unlike forward stepwise selection, it begins with the full least squares model containing all p predictors, and then iteratively removes the least useful predictor, one-at-a-time. Details are given in Algorithm 6.3.

Algorithm 6.3 *Backward stepwise selection*

1. Let $\mathcal{M}_p$ denote the *full* model, which contains all p predictors.
2. For $k = p, p-1, \ldots, 1$:
   (a) Consider all k models that contain all but one of the predictors in $\mathcal{M}_k$, for a total of $k-1$ predictors.
   (b) Choose the *best* among these k models, and call it $\mathcal{M}_{k-1}$. Here *best* is defined as having smallest RSS or highest R^2.
3. Select a single best model from among $\mathcal{M}_0, \ldots, \mathcal{M}_p$ using the prediction error on a validation set, C_p (AIC), BIC, or adjusted R^2. Or use the cross-validation method.

Like forward stepwise selection, the backward selection approach searches through only $1 + p(p+1)/2$ models, and so can be applied in settings where

p is too large to apply best subset selection.[3] Also like forward stepwise selection, backward stepwise selection is not guaranteed to yield the *best* model containing a subset of the p predictors.

Backward selection requires that the number of samples n is larger than the number of variables p (so that the full model can be fit). In contrast, forward stepwise can be used even when $n < p$, and so is the only viable subset method when p is very large.

Hybrid Approaches

The best subset, forward stepwise, and backward stepwise selection approaches generally give similar but not identical models. As another alternative, hybrid versions of forward and backward stepwise selection are available, in which variables are added to the model sequentially, in analogy to forward selection. However, after adding each new variable, the method may also remove any variables that no longer provide an improvement in the model fit. Such an approach attempts to more closely mimic best subset selection while retaining the computational advantages of forward and backward stepwise selection.

6.1.3 Choosing the Optimal Model

Best subset selection, forward selection, and backward selection result in the creation of a set of models, each of which contains a subset of the p predictors. To apply these methods, we need a way to determine which of these models is *best*. As we discussed in Section 6.1.1, the model containing all of the predictors will always have the smallest RSS and the largest R^2, since these quantities are related to the training error. Instead, we wish to choose a model with a low test error. As is evident here, and as we show in Chapter 2, the training error can be a poor estimate of the test error. Therefore, RSS and R^2 are not suitable for selecting the best model among a collection of models with different numbers of predictors.

In order to select the best model with respect to test error, we need to estimate this test error. There are two common approaches:

1. We can indirectly estimate test error by making an *adjustment* to the training error to account for the bias due to overfitting.

2. We can *directly* estimate the test error, using either a validation set approach or a cross-validation approach, as discussed in Chapter 5.

We consider both of these approaches below.

[3] Like forward stepwise selection, backward stepwise selection performs a *guided* search over model space, and so effectively considers substantially more than $1 + p(p + 1)/2$ models.

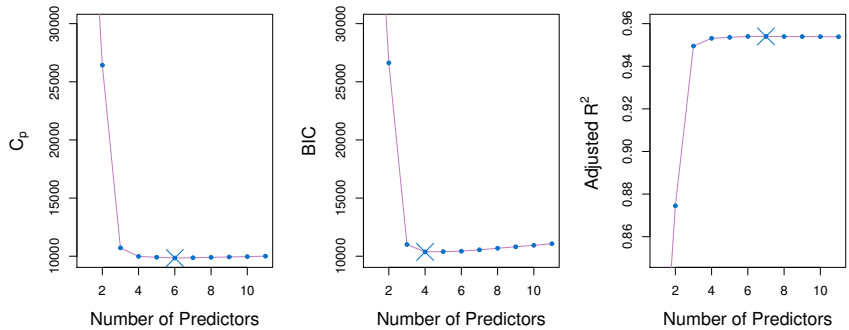


FIGURE 6.2. *C_p, BIC, and adjusted R^2 are shown for the best models of each size for the* `Credit` *data set (the lower frontier in Figure 6.1). C_p and BIC are estimates of test MSE. In the middle plot we see that the BIC estimate of test error shows an increase after four variables are selected. The other two plots are rather flat after four variables are included.*

C_p, AIC, BIC, and Adjusted R^2

We show in Chapter 2 that the training set MSE is generally an underestimate of the test MSE. (Recall that MSE $=$ RSS$/n$.) This is because when we fit a model to the training data using least squares, we specifically estimate the regression coefficients such that the training RSS (but not the test RSS) is as small as possible. In particular, the training error will decrease as more variables are included in the model, but the test error may not. Therefore, training set RSS and training set R^2 cannot be used to select from among a set of models with different numbers of variables.

However, a number of techniques for *adjusting* the training error for the model size are available. These approaches can be used to select among a set of models with different numbers of variables. We now consider four such approaches: C_p, *Akaike information criterion* (AIC), *Bayesian information criterion* (BIC), and *adjusted* R^2. Figure 6.2 displays C_p, BIC, and adjusted R^2 for the best model of each size produced by best subset selection on the `Credit` data set.

C_p
Akaike information criterion
Bayesian information criterion
adjusted R^2

For a fitted least squares model containing d predictors, the C_p estimate of test MSE is computed using the equation

$$C_p = \frac{1}{n}\left(\text{RSS} + 2d\hat{\sigma}^2\right), \tag{6.2}$$

where $\hat{\sigma}^2$ is an estimate of the variance of the error ϵ associated with each response measurement in (6.1).[4] Typically $\hat{\sigma}^2$ is estimated using the full

[4]Mallow's C_p is sometimes defined as $C_p' = \text{RSS}/\hat{\sigma}^2 + 2d - n$. This is equivalent to the definition given above in the sense that $C_p = \frac{1}{n}\hat{\sigma}^2(C_p' + n)$, and so the model with smallest C_p also has smallest C_p'.

model containing all predictors. Essentially, the C_p statistic adds a penalty of $2d\hat{\sigma}^2$ to the training RSS in order to adjust for the fact that the training error tends to underestimate the test error. Clearly, the penalty increases as the number of predictors in the model increases; this is intended to adjust for the corresponding decrease in training RSS. Though it is beyond the scope of this book, one can show that if $\hat{\sigma}^2$ is an unbiased estimate of σ^2 in (6.2), then C_p is an unbiased estimate of test MSE. As a consequence, the C_p statistic tends to take on a small value for models with a low test error, so when determining which of a set of models is best, we choose the model with the lowest C_p value. In Figure 6.2, C_p selects the six-variable model containing the predictors `income`, `limit`, `rating`, `cards`, `age` and `student`.

The AIC criterion is defined for a large class of models fit by maximum likelihood. In the case of the model (6.1) with Gaussian errors, maximum likelihood and least squares are the same thing. In this case AIC is given by

$$\text{AIC} = \frac{1}{n}\left(\text{RSS} + 2d\hat{\sigma}^2\right),$$

where, for simplicity, we have omitted irrelevant constants.[5] Hence for least squares models, C_p and AIC are proportional to each other, and so only C_p is displayed in Figure 6.2.

BIC is derived from a Bayesian point of view, but ends up looking similar to C_p (and AIC) as well. For the least squares model with d predictors, the BIC is, up to irrelevant constants, given by

$$\text{BIC} = \frac{1}{n}\left(\text{RSS} + \log(n)d\hat{\sigma}^2\right). \tag{6.3}$$

Like C_p, the BIC will tend to take on a small value for a model with a low test error, and so generally we select the model that has the lowest BIC value. Notice that BIC replaces the $2d\hat{\sigma}^2$ used by C_p with a $\log(n)d\hat{\sigma}^2$ term, where n is the number of observations. Since $\log n > 2$ for any $n > 7$, the BIC statistic generally places a heavier penalty on models with many variables, and hence results in the selection of smaller models than C_p. In Figure 6.2, we see that this is indeed the case for the `Credit` data set; BIC chooses a model that contains only the four predictors `income`, `limit`, `cards`, and `student`. In this case the curves are very flat and so there does not appear to be much difference in accuracy between the four-variable and six-variable models.

The adjusted R^2 statistic is another popular approach for selecting among a set of models that contain different numbers of variables. Recall from

[5]There are two formulas for AIC for least squares regression. The formula that we provide here requires an expression for σ^2, which we obtain using the full model containing all predictors. The second formula is appropriate when σ^2 is unknown and we do not want to explicitly estimate it; that formula has a log(RSS) term instead of an RSS term. Detailed derivations of these two formulas are outside of the scope of this book.

Chapter 3 that the usual R^2 is defined as $1 - \text{RSS}/\text{TSS}$, where $\text{TSS} = \sum(y_i - \overline{y})^2$ is the *total sum of squares* for the response. Since RSS always decreases as more variables are added to the model, the R^2 always increases as more variables are added. For a least squares model with d variables, the adjusted R^2 statistic is calculated as

$$\text{Adjusted } R^2 = 1 - \frac{\text{RSS}/(n-d-1)}{\text{TSS}/(n-1)}. \tag{6.4}$$

Unlike C_p, AIC, and BIC, for which a *small* value indicates a model with a low test error, a *large* value of adjusted R^2 indicates a model with a small test error. Maximizing the adjusted R^2 is equivalent to minimizing $\frac{\text{RSS}}{n-d-1}$. While RSS always decreases as the number of variables in the model increases, $\frac{\text{RSS}}{n-d-1}$ may increase or decrease, due to the presence of d in the denominator.

The intuition behind the adjusted R^2 is that once all of the correct variables have been included in the model, adding additional *noise* variables will lead to only a very small decrease in RSS. Since adding noise variables leads to an increase in d, such variables will lead to an increase in $\frac{\text{RSS}}{n-d-1}$, and consequently a decrease in the adjusted R^2. Therefore, in theory, the model with the largest adjusted R^2 will have only correct variables and no noise variables. Unlike the R^2 statistic, the adjusted R^2 statistic *pays a price* for the inclusion of unnecessary variables in the model. Figure 6.2 displays the adjusted R^2 for the `Credit` data set. Using this statistic results in the selection of a model that contains seven variables, adding `own` to the model selected by C_p and AIC.

C_p, AIC, and BIC all have rigorous theoretical justifications that are beyond the scope of this book. These justifications rely on asymptotic arguments (scenarios where the sample size n is very large). Despite its popularity, and even though it is quite intuitive, the adjusted R^2 is not as well motivated in statistical theory as AIC, BIC, and C_p. All of these measures are simple to use and compute. Here we have presented their formulas in the case of a linear model fit using least squares; however, AIC and BIC can also be defined for more general types of models.

Validation and Cross-Validation

As an alternative to the approaches just discussed, we can directly estimate the test error using the validation set and cross-validation methods discussed in Chapter 5. We can compute the validation set error or the cross-validation error for each model under consideration, and then select the model for which the resulting estimated test error is smallest. This procedure has an advantage relative to AIC, BIC, C_p, and adjusted R^2, in that it provides a direct estimate of the test error, and makes fewer assumptions about the true underlying model. It can also be used in a wider range of model selection tasks, even in cases where it is hard to pinpoint the model

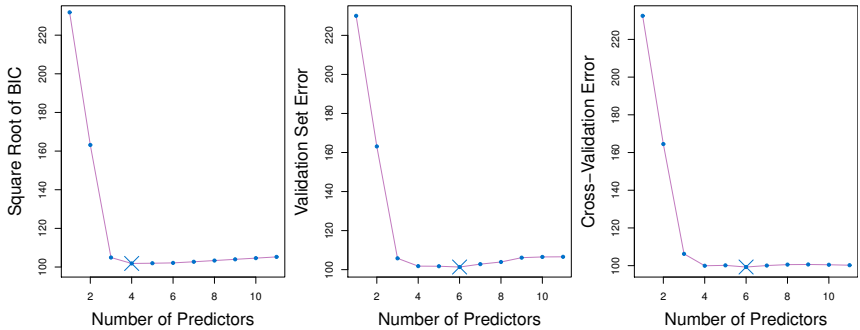


FIGURE 6.3. *For the* `Credit` *data set, three quantities are displayed for the best model containing d predictors, for d ranging from* 1 *to* 11. *The overall* best *model, based on each of these quantities, is shown as a blue cross.* Left: *Square root of BIC.* Center: *Validation set errors.* Right: *Cross-validation errors.*

degrees of freedom (e.g. the number of predictors in the model) or hard to estimate the error variance σ^2. Note that when cross-validation is used, the sequence of models $\mathcal{M}_k$ in Algorithms 6.1–6.3 is determined separately for each training fold, and the validation errors are averaged over all folds for each model size k. This means, for example with best-subset regression, that $\mathcal{M}_k$, the best subset of size k, can differ across the folds. Once the best size k is chosen, we find the best model of that size on the full data set.

In the past, performing cross-validation was computationally prohibitive for many problems with large p and/or large n, and so AIC, BIC, C_p, and adjusted R^2 were more attractive approaches for choosing among a set of models. However, nowadays with fast computers, the computations required to perform cross-validation are hardly ever an issue. Thus, cross-validation is a very attractive approach for selecting from among a number of models under consideration.

Figure 6.3 displays, as a function of d, the BIC, validation set errors, and cross-validation errors on the `Credit` data, for the best d-variable model. The validation errors were calculated by randomly selecting three-quarters of the observations as the training set, and the remainder as the validation set. The cross-validation errors were computed using $k = 10$ folds. In this case, the validation and cross-validation methods both result in a six-variable model. However, all three approaches suggest that the four-, five-, and six-variable models are roughly equivalent in terms of their test errors.

In fact, the estimated test error curves displayed in the center and right-hand panels of Figure 6.3 are quite flat. While a three-variable model clearly has lower estimated test error than a two-variable model, the estimated test errors of the 3- to 11-variable models are quite similar. Furthermore, if we

repeated the validation set approach using a different split of the data into a training set and a validation set, or if we repeated cross-validation using a different set of cross-validation folds, then the precise model with the lowest estimated test error would surely change. In this setting, we can select a model using the *one-standard-error rule*. We first calculate the standard error of the estimated test MSE for each model size, and then select the smallest model for which the estimated test error is within one standard error of the lowest point on the curve. The rationale here is that if a set of models appear to be more or less equally good, then we might as well choose the simplest model—that is, the model with the smallest number of predictors. In this case, applying the one-standard-error rule to the validation set or cross-validation approach leads to selection of the three-variable model.

one-standard-error rule

6.2 Shrinkage Methods

The subset selection methods described in Section 6.1 involve using least squares to fit a linear model that contains a subset of the predictors. As an alternative, we can fit a model containing all p predictors using a technique that *constrains* or *regularizes* the coefficient estimates, or equivalently, that *shrinks* the coefficient estimates towards zero. It may not be immediately obvious why such a constraint should improve the fit, but it turns out that shrinking the coefficient estimates can significantly reduce their variance. The two best-known techniques for shrinking the regression coefficients towards zero are *ridge regression* and the *lasso*.

6.2.1 Ridge Regression

Recall from Chapter 3 that the least squares fitting procedure estimates $\beta_0, \beta_1, \ldots, \beta_p$ using the values that minimize

$$\text{RSS} = \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij} \right)^2 .$$

Ridge regression is very similar to least squares, except that the coefficients are estimated by minimizing a slightly different quantity. In particular, the ridge regression coefficient estimates $\hat{\beta}^R$ are the values that minimize

ridge regression

$$\sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij} \right)^2 + \lambda \sum_{j=1}^{p} \beta_j^2 = \text{RSS} + \lambda \sum_{j=1}^{p} \beta_j^2, \tag{6.5}$$

where $\lambda \geq 0$ is a *tuning parameter*, to be determined separately. Equa-

tuning parameter

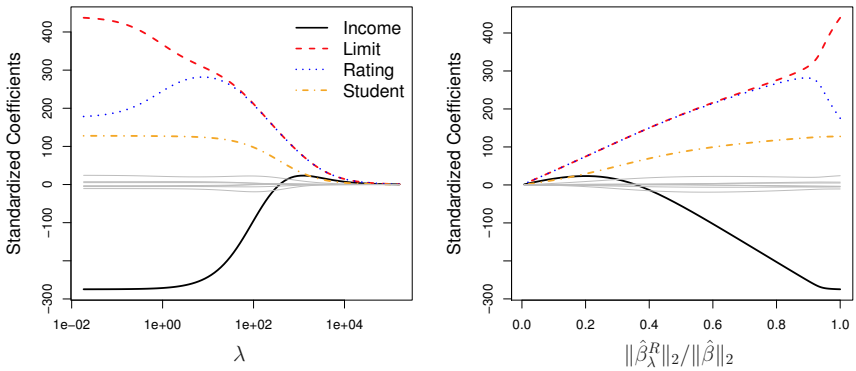


FIGURE 6.4. *The standardized ridge regression coefficients are displayed for the* `Credit` *data set, as a function of* λ *and* $\|\hat{\beta}_\lambda^R\|_2/\|\hat{\beta}\|_2$.

tion 6.5 trades off two different criteria. As with least squares, ridge regression seeks coefficient estimates that fit the data well, by making the RSS small. However, the second term, $\lambda \sum_j \beta_j^2$, called a *shrinkage penalty*, is small when $\beta_1, \ldots, \beta_p$ are close to zero, and so it has the effect of *shrinking* the estimates of β_j towards zero. The tuning parameter λ serves to control the relative impact of these two terms on the regression coefficient estimates. When $\lambda = 0$, the penalty term has no effect, and ridge regression will produce the least squares estimates. However, as $\lambda \to \infty$, the impact of the shrinkage penalty grows, and the ridge regression coefficient estimates will approach zero. Unlike least squares, which generates only one set of coefficient estimates, ridge regression will produce a different set of coefficient estimates, $\hat{\beta}_\lambda^R$, for each value of λ. Selecting a good value for λ is critical; we defer this discussion to Section 6.2.3, where we use cross-validation.

shrinkage penalty

Note that in (6.5), the shrinkage penalty is applied to $\beta_1, \ldots, \beta_p$, but not to the intercept β_0. We want to shrink the estimated association of each variable with the response; however, we do not want to shrink the intercept, which is simply a measure of the mean value of the response when $x_{i1} = x_{i2} = \ldots = x_{ip} = 0$. If we assume that the variables—that is, the columns of the data matrix $\mathbf{X}$—have been centered to have mean zero before ridge regression is performed, then the estimated intercept will take the form $\hat{\beta}_0 = \bar{y} = \sum_{i=1}^n y_i/n$.

An Application to the Credit Data

In Figure 6.4, the ridge regression coefficient estimates for the `Credit` data set are displayed. In the left-hand panel, each curve corresponds to the ridge regression coefficient estimate for one of the ten variables, plotted as a function of λ. For example, the black solid line represents the ridge regression estimate for the `income` coefficient, as λ is varied. At the extreme

left-hand side of the plot, λ is essentially zero, and so the corresponding ridge coefficient estimates are the same as the usual least squares estimates. But as λ increases, the ridge coefficient estimates shrink towards zero. When λ is extremely large, then all of the ridge coefficient estimates are basically zero; this corresponds to the *null model* that contains no predictors. In this plot, the `income`, `limit`, `rating`, and `student` variables are displayed in distinct colors, since these variables tend to have by far the largest coefficient estimates. While the ridge coefficient estimates tend to decrease in aggregate as λ increases, individual coefficients, such as `rating` and `income`, may occasionally increase as λ increases.

The right-hand panel of Figure 6.4 displays the same ridge coefficient estimates as the left-hand panel, but instead of displaying λ on the x-axis, we now display $\|\hat{\beta}_\lambda^R\|_2/\|\hat{\beta}\|_2$, where $\hat{\beta}$ denotes the vector of least squares coefficient estimates. The notation $\|\beta\|_2$ denotes the ℓ_2 *norm* (pronounced "ell 2") of a vector, and is defined as $\|\beta\|_2 = \sqrt{\sum_{j=1}^{p} \beta_j{}^2}$. It measures the distance of β from zero. As λ increases, the ℓ_2 norm of $\hat{\beta}_\lambda^R$ will *always* decrease, and so will $\|\hat{\beta}_\lambda^R\|_2/\|\hat{\beta}\|_2$. The latter quantity ranges from 1 (when $\lambda = 0$, in which case the ridge regression coefficient estimate is the same as the least squares estimate, and so their ℓ_2 norms are the same) to 0 (when $\lambda = \infty$, in which case the ridge regression coefficient estimate is a vector of zeros, with ℓ_2 norm equal to zero). Therefore, we can think of the x-axis in the right-hand panel of Figure 6.4 as the amount that the ridge regression coefficient estimates have been shrunken towards zero; a small value indicates that they have been shrunken very close to zero.

ℓ_2 norm

The standard least squares coefficient estimates discussed in Chapter 3 are *scale equivariant*: multiplying X_j by a constant c simply leads to a scaling of the least squares coefficient estimates by a factor of $1/c$. In other words, regardless of how the jth predictor is scaled, $X_j\hat{\beta}_j$ will remain the same. In contrast, the ridge regression coefficient estimates can change *substantially* when multiplying a given predictor by a constant. For instance, consider the `income` variable, which is measured in dollars. One could reasonably have measured income in thousands of dollars, which would result in a reduction in the observed values of `income` by a factor of 1,000. Now due to the sum of squared coefficients term in the ridge regression formulation (6.5), such a change in scale will not simply cause the ridge regression coefficient estimate for `income` to change by a factor of 1,000. In other words, $X_j\hat{\beta}_{j,\lambda}^R$ will depend not only on the value of λ, but also on the scaling of the jth predictor. In fact, the value of $X_j\hat{\beta}_{j,\lambda}^R$ may even depend on the scaling of the *other* predictors! Therefore, it is best to apply ridge regression after *standardizing the predictors*, using the formula

scale equivariant

$$\tilde{x}_{ij} = \frac{x_{ij}}{\sqrt{\frac{1}{n}\sum_{i=1}^{n}(x_{ij} - \overline{x}_j)^2}}, \tag{6.6}$$

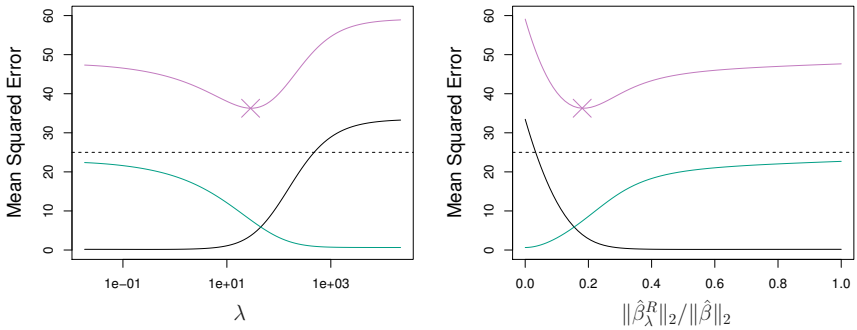


FIGURE 6.5. *Squared bias (black), variance (green), and test mean squared error (purple) for the ridge regression predictions on a simulated data set, as a function of* λ *and* $\|\hat{\beta}^R_\lambda\|_2/\|\hat{\beta}\|_2$*. The horizontal dashed lines indicate the minimum possible MSE. The purple crosses indicate the ridge regression models for which the MSE is smallest.*

so that they are all on the same scale. In (6.6), the denominator is the estimated standard deviation of the jth predictor. Consequently, all of the standardized predictors will have a standard deviation of one. As a result the final fit will not depend on the scale on which the predictors are measured. In Figure 6.4, the y-axis displays the standardized ridge regression coefficient estimates—that is, the coefficient estimates that result from performing ridge regression using standardized predictors.

Why Does Ridge Regression Improve Over Least Squares?

Ridge regression's advantage over least squares is rooted in the *bias-variance trade-off*. As λ increases, the flexibility of the ridge regression fit decreases, leading to decreased variance but increased bias. This is illustrated in the left-hand panel of Figure 6.5, using a simulated data set containing $p = 45$ predictors and $n = 50$ observations. The green curve in the left-hand panel of Figure 6.5 displays the variance of the ridge regression predictions as a function of λ. At the least squares coefficient estimates, which correspond to ridge regression with $\lambda = 0$, the variance is high but there is no bias. But as λ increases, the shrinkage of the ridge coefficient estimates leads to a substantial reduction in the variance of the predictions, at the expense of a slight increase in bias. Recall that the test mean squared error (MSE), plotted in purple, is closely related to the variance plus the squared bias. For values of λ up to about 10, the variance decreases rapidly, with very little increase in bias, plotted in black. Consequently, the MSE drops considerably as λ increases from 0 to 10. Beyond this point, the decrease in variance due to increasing λ slows, and the shrinkage on the coefficients causes them to be significantly underestimated, resulting in a large increase in the bias. The minimum MSE is achieved at approximately $\lambda = 30$. Interestingly,

because of its high variance, the MSE associated with the least squares fit, when $\lambda = 0$, is almost as high as that of the null model for which all coefficient estimates are zero, when $\lambda = \infty$. However, for an intermediate value of λ, the MSE is considerably lower.

The right-hand panel of Figure 6.5 displays the same curves as the left-hand panel, this time plotted against the ℓ_2 norm of the ridge regression coefficient estimates divided by the ℓ_2 norm of the least squares estimates. Now as we move from left to right, the fits become more flexible, and so the bias decreases and the variance increases.

In general, in situations where the relationship between the response and the predictors is close to linear, the least squares estimates will have low bias but may have high variance. This means that a small change in the training data can cause a large change in the least squares coefficient estimates. In particular, when the number of variables p is almost as large as the number of observations n, as in the example in Figure 6.5, the least squares estimates will be extremely variable. And if $p > n$, then the least squares estimates do not even have a unique solution, whereas ridge regression can still perform well by trading off a small increase in bias for a large decrease in variance. Hence, ridge regression works best in situations where the least squares estimates have high variance.

Ridge regression also has substantial computational advantages over best subset selection, which requires searching through 2^p models. As we discussed previously, even for moderate values of p, such a search can be computationally infeasible. In contrast, for any fixed value of λ, ridge regression only fits a single model, and the model-fitting procedure can be performed quite quickly. In fact, one can show that the computations required to solve (6.5), *simultaneously for all values of* λ, are almost identical to those for fitting a model using least squares.

6.2.2 The Lasso

Ridge regression does have one obvious disadvantage. Unlike best subset, forward stepwise, and backward stepwise selection, which will generally select models that involve just a subset of the variables, ridge regression will include all p predictors in the final model. The penalty $\lambda \sum \beta_j^2$ in (6.5) will shrink all of the coefficients towards zero, but it will not set any of them exactly to zero (unless $\lambda = \infty$). This may not be a problem for prediction accuracy, but it can create a challenge in model interpretation in settings in which the number of variables p is quite large. For example, in the `Credit` data set, it appears that the most important variables are `income`, `limit`, `rating`, and `student`. So we might wish to build a model including just these predictors. However, ridge regression will always generate a model involving all ten predictors. Increasing the value of λ will tend to reduce the magnitudes of the coefficients, but will not result in exclusion of any of the variables.

The *lasso* is a relatively recent alternative to ridge regression that overcomes this disadvantage. The lasso coefficients, $\hat{\beta}_\lambda^L$, minimize the quantity lasso

$$\sum_{i=1}^{n}\left(y_i - \beta_0 - \sum_{j=1}^{p}\beta_j x_{ij}\right)^2 + \lambda\sum_{j=1}^{p}|\beta_j| = \text{RSS} + \lambda\sum_{j=1}^{p}|\beta_j|. \quad (6.7)$$

Comparing (6.7) to (6.5), we see that the lasso and ridge regression have similar formulations. The only difference is that the β_j^2 term in the ridge regression penalty (6.5) has been replaced by $|\beta_j|$ in the lasso penalty (6.7). In statistical parlance, the lasso uses an ℓ_1 (pronounced "ell 1") penalty instead of an ℓ_2 penalty. The ℓ_1 norm of a coefficient vector β is given by $\|\beta\|_1 = \sum|\beta_j|$.

As with ridge regression, the lasso shrinks the coefficient estimates towards zero. However, in the case of the lasso, the ℓ_1 penalty has the effect of forcing some of the coefficient estimates to be exactly equal to zero when the tuning parameter λ is sufficiently large. Hence, much like best subset selection, the lasso performs *variable selection*. As a result, models generated from the lasso are generally much easier to interpret than those produced by ridge regression. We say that the lasso yields *sparse* models—that is, models that involve only a subset of the variables. As in ridge regression, selecting a good value of λ for the lasso is critical; we defer this discussion to Section 6.2.3, where we use cross-validation. sparse

As an example, consider the coefficient plots in Figure 6.6, which are generated from applying the lasso to the `Credit` data set. When $\lambda = 0$, then the lasso simply gives the least squares fit, and when λ becomes sufficiently large, the lasso gives the null model in which all coefficient estimates equal zero. However, in between these two extremes, the ridge regression and lasso models are quite different from each other. Moving from left to right in the right-hand panel of Figure 6.6, we observe that at first the lasso results in a model that contains only the `rating` predictor. Then `student` and `limit` enter the model almost simultaneously, shortly followed by `income`. Eventually, the remaining variables enter the model. Hence, depending on the value of λ, the lasso can produce a model involving any number of variables. In contrast, ridge regression will always include all of the variables in the model, although the magnitude of the coefficient estimates will depend on λ.

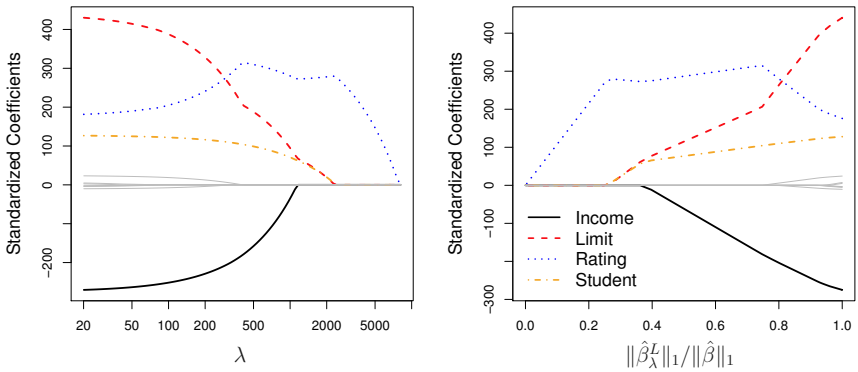


FIGURE 6.6. *The standardized lasso coefficients on the* `Credit` *data set are shown as a function of* λ *and* $\|\hat{\beta}_\lambda^L\|_1/\|\hat{\beta}\|_1$.

Another Formulation for Ridge Regression and the Lasso

One can show that the lasso and ridge regression coefficient estimates solve the problems

$$\underset{\beta}{\text{minimize}} \left\{ \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij} \right)^2 \right\} \quad \text{subject to} \quad \sum_{j=1}^{p} |\beta_j| \leq s \tag{6.8}$$

and

$$\underset{\beta}{\text{minimize}} \left\{ \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij} \right)^2 \right\} \quad \text{subject to} \quad \sum_{j=1}^{p} \beta_j^2 \leq s, \tag{6.9}$$

respectively. In other words, for every value of λ, there is some s such that the Equations (6.7) and (6.8) will give the same lasso coefficient estimates. Similarly, for every value of λ there is a corresponding s such that Equations (6.5) and (6.9) will give the same ridge regression coefficient estimates. When $p = 2$, then (6.8) indicates that the lasso coefficient estimates have the smallest RSS out of all points that lie within the diamond defined by $|\beta_1| + |\beta_2| \leq s$. Similarly, the ridge regression estimates have the smallest RSS out of all points that lie within the circle defined by $\beta_1^2 + \beta_2^2 \leq s$.

We can think of (6.8) as follows. When we perform the lasso we are trying to find the set of coefficient estimates that lead to the smallest RSS, subject to the constraint that there is a *budget* s for how large $\sum_{j=1}^{p} |\beta_j|$ can be. When s is extremely large, then this budget is not very restrictive, and so the coefficient estimates can be large. In fact, if s is large enough that the least squares solution falls within the budget, then (6.8) will simply yield the least squares solution. In contrast, if s is small, then $\sum_{j=1}^{p} |\beta_j|$ must be

small in order to avoid violating the budget. Similarly, (6.9) indicates that when we perform ridge regression, we seek a set of coefficient estimates such that the RSS is as small as possible, subject to the requirement that $\sum_{j=1}^{p} \beta_j^2$ not exceed the budget s.

The formulations (6.8) and (6.9) reveal a close connection between the lasso, ridge regression, and best subset selection. Consider the problem

$$\underset{\beta}{\text{minimize}} \left\{ \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij} \right)^2 \right\} \quad \text{subject to} \quad \sum_{j=1}^{p} I(\beta_j \neq 0) \leq s. \tag{6.10}$$

Here $I(\beta_j \neq 0)$ is an indicator variable: it takes on a value of 1 if $\beta_j \neq 0$, and equals zero otherwise. Then (6.10) amounts to finding a set of coefficient estimates such that RSS is as small as possible, subject to the constraint that no more than s coefficients can be nonzero. The problem (6.10) is equivalent to best subset selection. Unfortunately, solving (6.10) is computationally infeasible when p is large, since it requires considering all $\binom{p}{s}$ models containing s predictors. Therefore, we can interpret ridge regression and the lasso as computationally feasible alternatives to best subset selection that replace the intractable form of the budget in (6.10) with forms that are much easier to solve. Of course, the lasso is much more closely related to best subset selection, since the lasso performs feature selection for s sufficiently small in (6.8), while ridge regression does not.

The Variable Selection Property of the Lasso

Why is it that the lasso, unlike ridge regression, results in coefficient estimates that are exactly equal to zero? The formulations (6.8) and (6.9) can be used to shed light on the issue. Figure 6.7 illustrates the situation. The least squares solution is marked as $\hat{\beta}$, while the blue diamond and circle represent the lasso and ridge regression constraints in (6.8) and (6.9), respectively. If s is sufficiently large, then the constraint regions will contain $\hat{\beta}$, and so the ridge regression and lasso estimates will be the same as the least squares estimates. (Such a large value of s corresponds to $\lambda = 0$ in (6.5) and (6.7).) However, in Figure 6.7 the least squares estimates lie outside of the diamond and the circle, and so the least squares estimates are not the same as the lasso and ridge regression estimates.

Each of the ellipses centered around $\hat{\beta}$ represents a *contour*: this means that all of the points on a particular ellipse have the same RSS value. As the ellipses expand away from the least squares coefficient estimates, the RSS increases. Equations (6.8) and (6.9) indicate that the lasso and ridge regression coefficient estimates are given by the first point at which an ellipse contacts the constraint region. Since ridge regression has a circular constraint with no sharp points, this intersection will not generally occur on an axis, and so the ridge regression coefficient estimates will be exclusively

contour

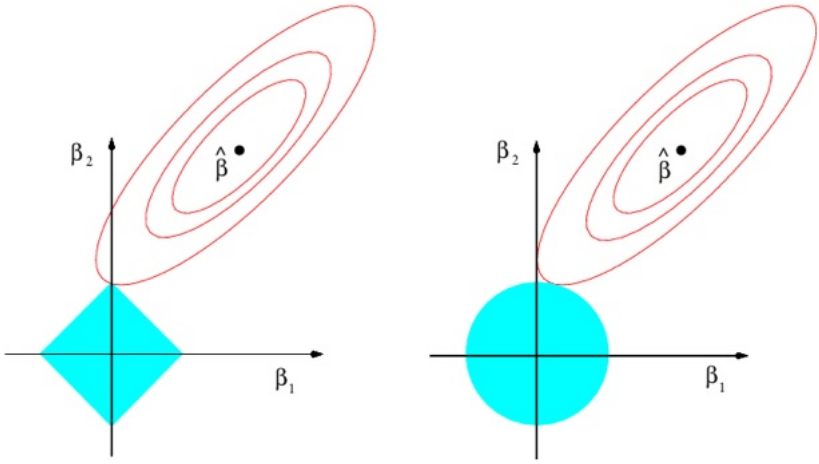


FIGURE 6.7. *Contours of the error and constraint functions for the lasso* (left) *and ridge regression* (right). *The solid blue areas are the constraint regions,* $|\beta_1| + |\beta_2| \leq s$ *and* $\beta_1^2 + \beta_2^2 \leq s$, *while the red ellipses are the contours of the RSS.*

non-zero. However, the lasso constraint has *corners* at each of the axes, and so the ellipse will often intersect the constraint region at an axis. When this occurs, one of the coefficients will equal zero. In higher dimensions, many of the coefficient estimates may equal zero simultaneously. In Figure 6.7, the intersection occurs at $\beta_1 = 0$, and so the resulting model will only include β_2.

In Figure 6.7, we considered the simple case of $p = 2$. When $p = 3$, then the constraint region for ridge regression becomes a sphere, and the constraint region for the lasso becomes a polyhedron. When $p > 3$, the constraint for ridge regression becomes a hypersphere, and the constraint for the lasso becomes a polytope. However, the key ideas depicted in Figure 6.7 still hold. In particular, the lasso leads to feature selection when $p > 2$ due to the sharp corners of the polyhedron or polytope.

Comparing the Lasso and Ridge Regression

It is clear that the lasso has a major advantage over ridge regression, in that it produces simpler and more interpretable models that involve only a subset of the predictors. However, which method leads to better prediction accuracy? Figure 6.8 displays the variance, squared bias, and test MSE of the lasso applied to the same simulated data as in Figure 6.5. Clearly the lasso leads to qualitatively similar behavior to ridge regression, in that as λ increases, the variance decreases and the bias increases. In the right-hand panel of Figure 6.8, the dotted lines represent the ridge regression fits. Here we plot both against their R^2 on the training data. This is another

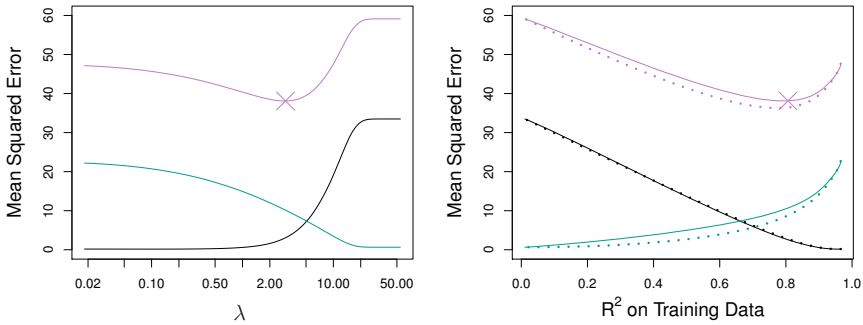


FIGURE 6.8. Left: *Plots of squared bias (black), variance (green), and test MSE (purple) for the lasso on a simulated data set.* Right: *Comparison of squared bias, variance, and test MSE between lasso (solid) and ridge (dotted). Both are plotted against their* R^2 *on the training data, as a common form of indexing. The crosses in both plots indicate the lasso model for which the MSE is smallest.*

useful way to index models, and can be used to compare models with different types of regularization, as is the case here. In this example, the lasso and ridge regression result in almost identical biases. However, the variance of ridge regression is slightly lower than the variance of the lasso. Consequently, the minimum MSE of ridge regression is slightly smaller than that of the lasso.

However, the data in Figure 6.8 were generated in such a way that all 45 predictors were related to the response—that is, none of the true coefficients $\beta_1, \ldots, \beta_{45}$ equaled zero. The lasso implicitly assumes that a number of the coefficients truly equal zero. Consequently, it is not surprising that ridge regression outperforms the lasso in terms of prediction error in this setting. Figure 6.9 illustrates a similar situation, except that now the response is a function of only 2 out of 45 predictors. Now the lasso tends to outperform ridge regression in terms of bias, variance, and MSE.

These two examples illustrate that neither ridge regression nor the lasso will universally dominate the other. In general, one might expect the lasso to perform better in a setting where a relatively small number of predictors have substantial coefficients, and the remaining predictors have coefficients that are very small or that equal zero. Ridge regression will perform better when the response is a function of many predictors, all with coefficients of roughly equal size. However, the number of predictors that is related to the response is never known *a priori* for real data sets. A technique such as cross-validation can be used in order to determine which approach is better on a particular data set.

As with ridge regression, when the least squares estimates have excessively high variance, the lasso solution can yield a reduction in variance at the expense of a small increase in bias, and consequently can gener-

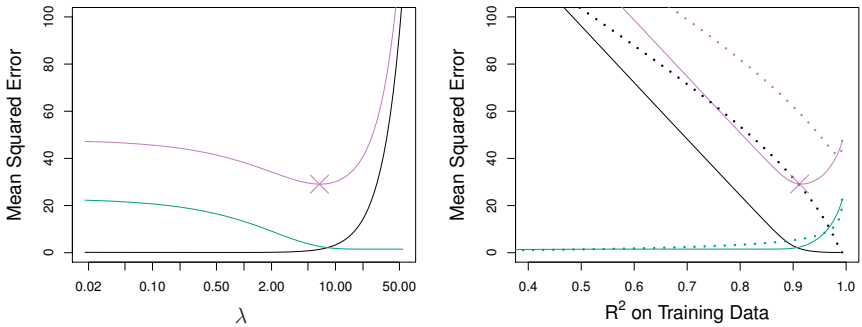


FIGURE 6.9. Left: *Plots of squared bias (black), variance (green), and test MSE (purple) for the lasso. The simulated data is similar to that in Figure 6.8, except that now only two predictors are related to the response.* Right: *Comparison of squared bias, variance, and test MSE between lasso (solid) and ridge (dotted). Both are plotted against their* R^2 *on the training data, as a common form of indexing. The crosses in both plots indicate the lasso model for which the MSE is smallest.*

ate more accurate predictions. Unlike ridge regression, the lasso performs variable selection, and hence results in models that are easier to interpret.

There are very efficient algorithms for fitting both ridge and lasso models; in both cases the entire coefficient paths can be computed with about the same amount of work as a single least squares fit. We will explore this further in the lab at the end of this chapter.

A Simple Special Case for Ridge Regression and the Lasso

In order to obtain a better intuition about the behavior of ridge regression and the lasso, consider a simple special case with $n = p$, and $\mathbf{X}$ a diagonal matrix with 1's on the diagonal and 0's in all off-diagonal elements. To simplify the problem further, assume also that we are performing regression without an intercept. With these assumptions, the usual least squares problem simplifies to finding $\beta_1, \ldots, \beta_p$ that minimize

$$\sum_{j=1}^{p}(y_j - \beta_j)^2. \tag{6.11}$$

In this case, the least squares solution is given by

$$\hat{\beta}_j = y_j.$$

And in this setting, ridge regression amounts to finding $\beta_1, \ldots, \beta_p$ such that

$$\sum_{j=1}^{p}(y_j - \beta_j)^2 + \lambda\sum_{j=1}^{p}\beta_j^2 \tag{6.12}$$

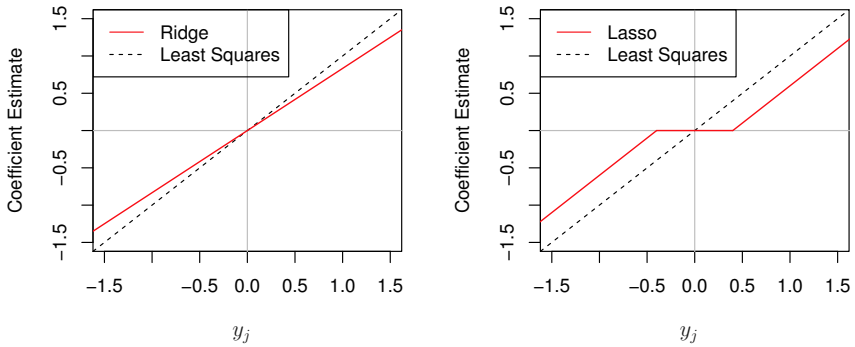


FIGURE 6.10. *The ridge regression and lasso coefficient estimates for a simple setting with $n = p$ and $\mathbf{X}$ a diagonal matrix with 1's on the diagonal.* Left: *The ridge regression coefficient estimates are shrunken proportionally towards zero, relative to the least squares estimates.* Right: *The lasso coefficient estimates are soft-thresholded towards zero.*

is minimized, and the lasso amounts to finding the coefficients such that

$$\sum_{j=1}^{p}(y_j - \beta_j)^2 + \lambda \sum_{j=1}^{p} |\beta_j| \tag{6.13}$$

is minimized. One can show that in this setting, the ridge regression estimates take the form

$$\hat{\beta}_j^R = y_j/(1+\lambda), \tag{6.14}$$

and the lasso estimates take the form

$$\hat{\beta}_j^L = \begin{cases} y_j - \lambda/2 & \text{if } y_j > \lambda/2; \\ y_j + \lambda/2 & \text{if } y_j < -\lambda/2; \\ 0 & \text{if } |y_j| \leq \lambda/2. \end{cases} \tag{6.15}$$

Figure 6.10 displays the situation. We can see that ridge regression and the lasso perform two very different types of shrinkage. In ridge regression, each least squares coefficient estimate is shrunken by the same proportion. In contrast, the lasso shrinks each least squares coefficient towards zero by a constant amount, $\lambda/2$; the least squares coefficients that are less than $\lambda/2$ in absolute value are shrunken entirely to zero. The type of shrinkage performed by the lasso in this simple setting (6.15) is known as *soft-thresholding*. The fact that some lasso coefficients are shrunken entirely to zero explains why the lasso performs feature selection.

soft-thresholding

In the case of a more general data matrix $\mathbf{X}$, the story is a little more complicated than what is depicted in Figure 6.10, but the main ideas still hold approximately: ridge regression more or less shrinks every dimension of the data by the same proportion, whereas the lasso more or less shrinks

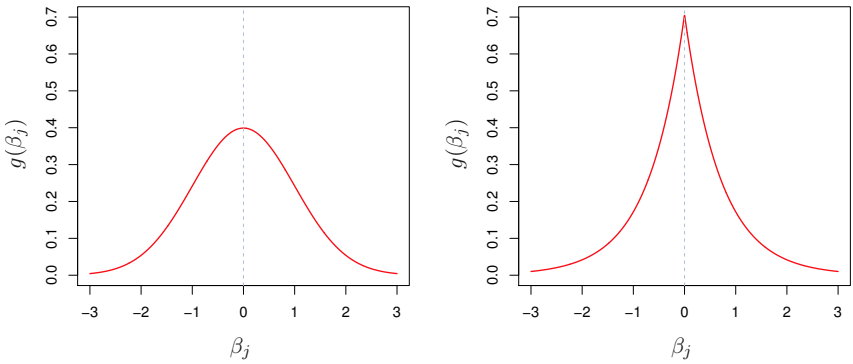


FIGURE 6.11. Left: *Ridge regression is the posterior mode for β under a Gaussian prior.* Right: *The lasso is the posterior mode for β under a double-exponential prior.*

all coefficients toward zero by a similar amount, and sufficiently small coefficients are shrunken all the way to zero.

Bayesian Interpretation of Ridge Regression and the Lasso

We now show that one can view ridge regression and the lasso through a Bayesian lens. A Bayesian viewpoint for regression assumes that the coefficient vector β has some *prior* distribution, say $p(\beta)$, where $\beta = (\beta_0, \beta_1, \ldots, \beta_p)^T$. The likelihood of the data can be written as $f(Y|X, \beta)$, where $X = (X_1, \ldots, X_p)$. Multiplying the prior distribution by the likelihood gives us (up to a proportionality constant) the *posterior distribution*, which takes the form

posterior distribution

$$p(\beta|X, Y) \propto f(Y|X, \beta)p(\beta|X) = f(Y|X, \beta)p(\beta),$$

where the proportionality above follows from Bayes' theorem, and the equality above follows from the assumption that X is fixed.

We assume the usual linear model,

$$Y = \beta_0 + X_1\beta_1 + \cdots + X_p\beta_p + \epsilon,$$

and suppose that the errors are independent and drawn from a normal distribution. Furthermore, assume that $p(\beta) = \prod_{j=1}^{p} g(\beta_j)$, for some density function g. It turns out that ridge regression and the lasso follow naturally from two special cases of g:

- If g is a Gaussian distribution with mean zero and standard deviation a function of λ, then it follows that the *posterior mode* for β—that is, the most likely value for β, given the data—is given by the ridge

posterior mode

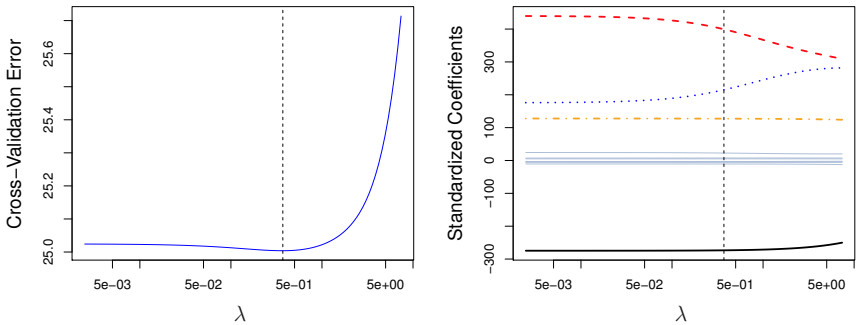


FIGURE 6.12. Left: *Cross-validation errors that result from applying ridge regression to the* `Credit` *data set with various values of* λ. Right: *The coefficient estimates as a function of* λ. *The vertical dashed lines indicate the value of* λ *selected by cross-validation.*

regression solution. (In fact, the ridge regression solution is also the posterior mean.)

- If g is a double-exponential (Laplace) distribution with mean zero and scale parameter a function of λ, then it follows that the posterior mode for β is the lasso solution. (However, the lasso solution is *not* the posterior mean, and in fact, the posterior mean does not yield a sparse coefficient vector.)

The Gaussian and double-exponential priors are displayed in Figure 6.11. Therefore, from a Bayesian viewpoint, ridge regression and the lasso follow directly from assuming the usual linear model with normal errors, together with a simple prior distribution for β. Notice that the lasso prior is steeply peaked at zero, while the Gaussian is flatter and fatter at zero. Hence, the lasso expects a priori that many of the coefficients are (exactly) zero, while ridge assumes the coefficients are randomly distributed about zero.

6.2.3 Selecting the Tuning Parameter

Just as the subset selection approaches considered in Section 6.1 require a method to determine which of the models under consideration is best, implementing ridge regression and the lasso requires a method for selecting a value for the tuning parameter λ in (6.5) and (6.7), or equivalently, the value of the constraint s in (6.9) and (6.8). Cross-validation provides a simple way to tackle this problem. We choose a grid of λ values, and compute the cross-validation error for each value of λ, as described in Chapter 5. We then select the tuning parameter value for which the cross-validation error is smallest. Finally, the model is re-fit using all of the available observations and the selected value of the tuning parameter.

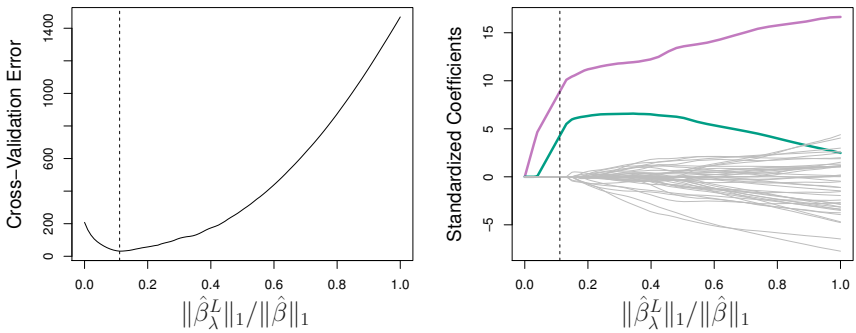


FIGURE 6.13. Left*: Ten-fold cross-validation MSE for the lasso, applied to the sparse simulated data set from Figure 6.9.* Right: *The corresponding lasso coefficient estimates are displayed. The two signal variables are shown in color, and the noise variables are in gray. The vertical dashed lines indicate the lasso fit for which the cross-validation error is smallest.*

Figure 6.12 displays the choice of λ that results from performing leave-one-out cross-validation on the ridge regression fits from the `Credit` data set. The dashed vertical lines indicate the selected value of λ. In this case the value is relatively small, indicating that the optimal fit only involves a small amount of shrinkage relative to the least squares solution. In addition, the dip is not very pronounced, so there is rather a wide range of values that would give a very similar error. In a case like this we might simply use the least squares solution.

Figure 6.13 provides an illustration of ten-fold cross-validation applied to the lasso fits on the sparse simulated data from Figure 6.9. The left-hand panel of Figure 6.13 displays the cross-validation error, while the right-hand panel displays the coefficient estimates. The vertical dashed lines indicate the point at which the cross-validation error is smallest. The two colored lines in the right-hand panel of Figure 6.13 represent the two predictors that are related to the response, while the grey lines represent the unrelated predictors; these are often referred to as *signal* and *noise* variables, respectively. Not only has the lasso correctly given much larger coefficient estimates to the two signal predictors, but also the minimum cross-validation error corresponds to a set of coefficient estimates for which only the signal variables are non-zero. Hence cross-validation together with the lasso has correctly identified the two signal variables in the model, even though this is a challenging setting, with $p = 45$ variables and only $n = 50$ observations. In contrast, the least squares solution—displayed on the far right of the right-hand panel of Figure 6.13—assigns a large coefficient estimate to only one of the two signal variables.

signal

6.3 Dimension Reduction Methods

The methods that we have discussed so far in this chapter have controlled variance in two different ways, either by using a subset of the original variables, or by shrinking their coefficients toward zero. All of these methods are defined using the original predictors, $X_1, X_2, \ldots, X_p$. We now explore a class of approaches that *transform* the predictors and then fit a least squares model using the transformed variables. We will refer to these techniques as *dimension reduction* methods.

dimension reduction
linear combination

Let $Z_1, Z_2, \ldots, Z_M$ represent $M < p$ *linear combinations* of our original p predictors. That is,

$$Z_m = \sum_{j=1}^{p} \phi_{jm} X_j \tag{6.16}$$

for some constants $\phi_{1m}, \phi_{2m} \ldots, \phi_{pm}$, $m = 1, \ldots, M$. We can then fit the linear regression model

$$y_i = \theta_0 + \sum_{m=1}^{M} \theta_m z_{im} + \epsilon_i, \quad i = 1, \ldots, n, \tag{6.17}$$

using least squares. Note that in (6.17), the regression coefficients are given by $\theta_0, \theta_1, \ldots, \theta_M$. If the constants $\phi_{1m}, \phi_{2m}, \ldots, \phi_{pm}$ are chosen wisely, then such dimension reduction approaches can often outperform least squares regression. In other words, fitting (6.17) using least squares can lead to better results than fitting (6.1) using least squares.

The term *dimension reduction* comes from the fact that this approach reduces the problem of estimating the $p+1$ coefficients $\beta_0, \beta_1, \ldots, \beta_p$ to the simpler problem of estimating the $M+1$ coefficients $\theta_0, \theta_1, \ldots, \theta_M$, where $M < p$. In other words, the dimension of the problem has been reduced from $p+1$ to $M+1$.

Notice that from (6.16),

$$\sum_{m=1}^{M} \theta_m z_{im} = \sum_{m=1}^{M} \theta_m \sum_{j=1}^{p} \phi_{jm} x_{ij} = \sum_{j=1}^{p} \sum_{m=1}^{M} \theta_m \phi_{jm} x_{ij} = \sum_{j=1}^{p} \beta_j x_{ij},$$

where

$$\beta_j = \sum_{m=1}^{M} \theta_m \phi_{jm}. \tag{6.18}$$

Hence (6.17) can be thought of as a special case of the original linear regression model given by (6.1). Dimension reduction serves to constrain the estimated β_j coefficients, since now they must take the form (6.18). This constraint on the form of the coefficients has the potential to bias the coefficient estimates. However, in situations where p is large relative to n, selecting a value of $M \ll p$ can significantly reduce the variance of the fitted

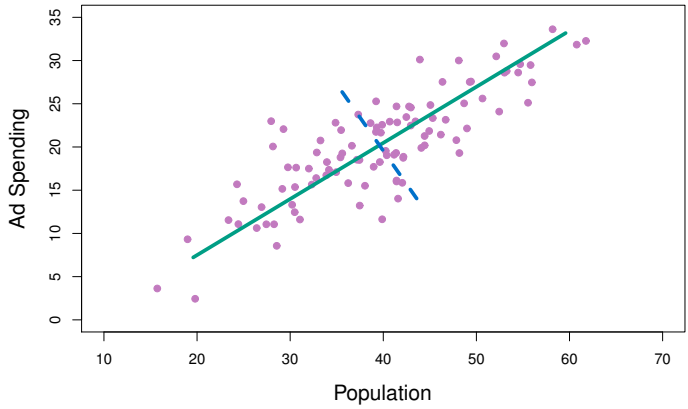


FIGURE 6.14. *The population size (*pop*) and ad spending (*ad*) for* 100 *different cities are shown as purple circles. The green solid line indicates the first principal component, and the blue dashed line indicates the second principal component.*

coefficients. If $M = p$, and all the Z_m are linearly independent, then (6.18) poses no constraints. In this case, no dimension reduction occurs, and so fitting (6.17) is equivalent to performing least squares on the original p predictors.

All dimension reduction methods work in two steps. First, the transformed predictors $Z_1, Z_2, \ldots, Z_M$ are obtained. Second, the model is fit using these M predictors. However, the choice of $Z_1, Z_2, \ldots, Z_M$, or equivalently, the selection of the ϕ_{jm}'s, can be achieved in different ways. In this chapter, we will consider two approaches for this task: *principal components* and *partial least squares*.

6.3.1 Principal Components Regression

Principal components analysis (PCA) is a popular approach for deriving a low-dimensional set of features from a large set of variables. PCA is discussed in greater detail as a tool for *unsupervised learning* in Chapter 12. Here we describe its use as a dimension reduction technique for regression.

principal components analysis

An Overview of Principal Components Analysis

PCA is a technique for reducing the dimension of an $n \times p$ data matrix $\mathbf{X}$. The *first principal component* direction of the data is that along which the observations *vary the most*. For instance, consider Figure 6.14, which shows population size (pop) in tens of thousands of people, and ad spending for a

particular company (ad) in thousands of dollars, for 100 cities.[6] The green solid line represents the first principal component direction of the data. We can see by eye that this is the direction along which there is the greatest variability in the data. That is, if we *projected* the 100 observations onto this line (as shown in the left-hand panel of Figure 6.15), then the resulting projected observations would have the largest possible variance; projecting the observations onto any other line would yield projected observations with lower variance. Projecting a point onto a line simply involves finding the location on the line which is closest to the point.

The first principal component is displayed graphically in Figure 6.14, but how can it be summarized mathematically? It is given by the formula

$$Z_1 = 0.839 \times (\texttt{pop} - \overline{\texttt{pop}}) + 0.544 \times (\texttt{ad} - \overline{\texttt{ad}}). \tag{6.19}$$

Here $\phi_{11} = 0.839$ and $\phi_{21} = 0.544$ are the principal component loadings, which define the direction referred to above. In (6.19), $\overline{\texttt{pop}}$ indicates the mean of all pop values in this data set, and $\overline{\texttt{ad}}$ indicates the mean of all advertising spending. The idea is that out of every possible *linear combination* of pop and ad such that $\phi_{11}^2 + \phi_{21}^2 = 1$, this particular linear combination yields the highest variance: i.e. this is the linear combination for which $\text{Var}(\phi_{11} \times (\texttt{pop} - \overline{\texttt{pop}}) + \phi_{21} \times (\texttt{ad} - \overline{\texttt{ad}}))$ is maximized. It is necessary to consider only linear combinations of the form $\phi_{11}^2 + \phi_{21}^2 = 1$, since otherwise we could increase ϕ_{11} and ϕ_{21} arbitrarily in order to blow up the variance. In (6.19), the two loadings are both positive and have similar size, and so Z_1 is almost an *average* of the two variables.

Since $n = 100$, pop and ad are vectors of length 100, and so is Z_1 in (6.19). For instance,

$$z_{i1} = 0.839 \times (\texttt{pop}_i - \overline{\texttt{pop}}) + 0.544 \times (\texttt{ad}_i - \overline{\texttt{ad}}). \tag{6.20}$$

The values of $z_{11}, \ldots, z_{n1}$ are known as the *principal component scores*, and can be seen in the right-hand panel of Figure 6.15.

There is also another interpretation of PCA: the first principal component vector defines the line that is *as close as possible* to the data. For instance, in Figure 6.14, the first principal component line minimizes the sum of the squared perpendicular distances between each point and the line. These distances are plotted as dashed line segments in the left-hand panel of Figure 6.15, in which the crosses represent the *projection* of each point onto the first principal component line. The first principal component has been chosen so that the projected observations are *as close as possible* to the original observations.

In the right-hand panel of Figure 6.15, the left-hand panel has been rotated so that the first principal component direction coincides with the x-axis. It is possible to show that the *first principal component score* for

[6] This dataset is distinct from the Advertising data discussed in Chapter 3.

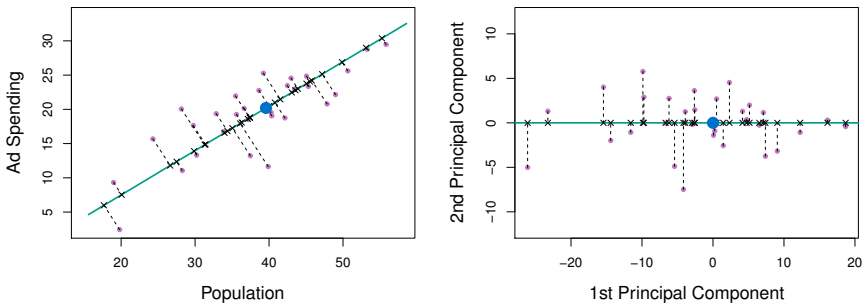


FIGURE 6.15. *A subset of the advertising data. The mean* pop *and* ad *budgets are indicated with a blue circle.* Left: *The first principal component direction is shown in green. It is the dimension along which the data vary the most, and it also defines the line that is closest to all n of the observations. The distances from each observation to the principal component are represented using the black dashed line segments. The blue dot represents* $(\overline{\texttt{pop}}, \overline{\texttt{ad}})$. Right: *The left-hand panel has been rotated so that the first principal component direction coincides with the x-axis.*

the ith observation, given in (6.20), is the distance in the x-direction of the ith cross from zero. So for example, the point in the bottom-left corner of the left-hand panel of Figure 6.15 has a large negative principal component score, $z_{i1} = -26.1$, while the point in the top-right corner has a large positive score, $z_{i1} = 18.7$. These scores can be computed directly using (6.20).

We can think of the values of the principal component Z_1 as single-number summaries of the joint pop and ad budgets for each location. In this example, if $z_{i1} = 0.839 \times (\texttt{pop}_i - \overline{\texttt{pop}}) + 0.544 \times (\texttt{ad}_i - \overline{\texttt{ad}}) < 0$, then this indicates a city with below-average population size and below-average ad spending. A positive score suggests the opposite. How well can a single number represent both pop and ad? In this case, Figure 6.14 indicates that pop and ad have approximately a linear relationship, and so we might expect that a single-number summary will work well. Figure 6.16 displays z_{i1} versus both pop and ad.[7] The plots show a strong relationship between the first principal component and the two features. In other words, the first principal component appears to capture most of the information contained in the pop and ad predictors.

So far we have concentrated on the first principal component. In general, one can construct up to p distinct principal components. The second principal component Z_2 is a linear combination of the variables that is uncorrelated with Z_1, and has largest variance subject to this constraint. The

[7]The principal components were calculated after first standardizing both pop and ad, a common approach. Hence, the x-axes on Figures 6.15 and 6.16 are not on the same scale.

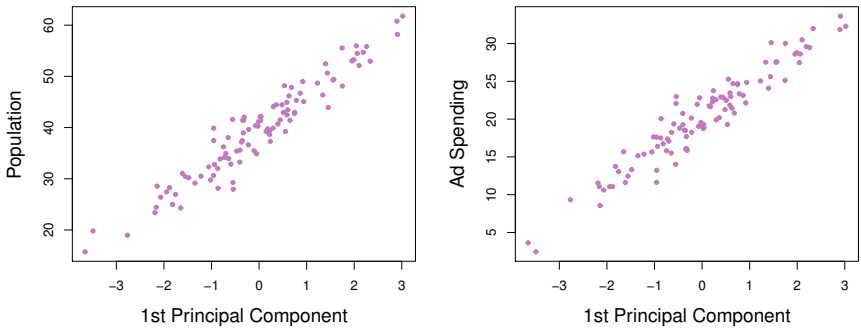


FIGURE 6.16. *Plots of the first principal component scores z_{i1} versus* pop *and* ad*. The relationships are strong.*

second principal component direction is illustrated as a dashed blue line in Figure 6.14. It turns out that the zero correlation condition of Z_1 with Z_2 is equivalent to the condition that the direction must be *perpendicular*, or *orthogonal*, to the first principal component direction. The second principal component is given by the formula

perpendicular
orthogonal

$$Z_2 = 0.544 \times (\texttt{pop} - \overline{\texttt{pop}}) - 0.839 \times (\texttt{ad} - \overline{\texttt{ad}}).$$

Since the advertising data has two predictors, the first two principal components contain all of the information that is in pop and ad. However, by construction, the first component will contain the most information. Consider, for example, the much larger variability of z_{i1} (the x-axis) versus z_{i2} (the y-axis) in the right-hand panel of Figure 6.15. The fact that the second principal component scores are much closer to zero indicates that this component captures far less information. As another illustration, Figure 6.17 displays z_{i2} versus pop and ad. There is little relationship between the second principal component and these two predictors, again suggesting that in this case, one only needs the first principal component in order to accurately represent the pop and ad budgets.

With two-dimensional data, such as in our advertising example, we can construct at most two principal components. However, if we had other predictors, such as population age, income level, education, and so forth, then additional components could be constructed. They would successively maximize variance, subject to the constraint of being uncorrelated with the preceding components.

The Principal Components Regression Approach

The *principal components regression* (PCR) approach involves constructing the first M principal components, $Z_1, \ldots, Z_M$, and then using these components as the predictors in a linear regression model that is fit using least squares. The key idea is that often a small number of principal

principal components regression

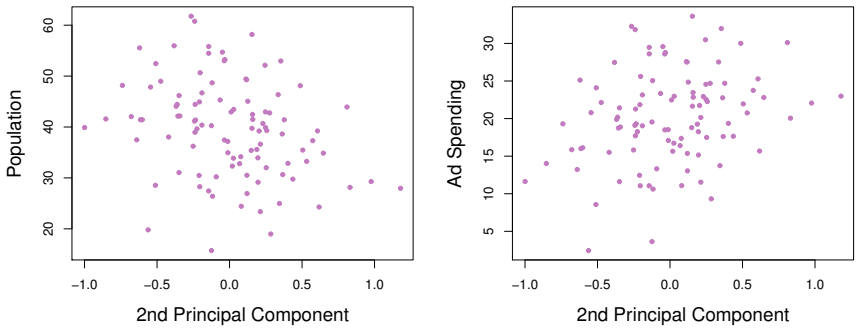


FIGURE 6.17. *Plots of the second principal component scores z_{i2} versus* pop *and* ad*. The relationships are weak.*

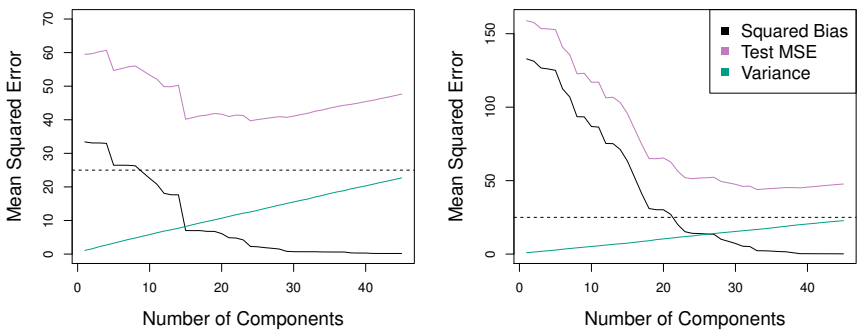


FIGURE 6.18. *PCR was applied to two simulated data sets. In each panel, the horizontal dashed line represents the irreducible error.* Left: *Simulated data from Figure 6.8.* Right: *Simulated data from Figure 6.9.*

components suffice to explain most of the variability in the data, as well as the relationship with the response. In other words, we assume that *the directions in which $X_1, \ldots, X_p$ show the most variation are the directions that are associated with Y*. While this assumption is not guaranteed to be true, it often turns out to be a reasonable enough approximation to give good results.

If the assumption underlying PCR holds, then fitting a least squares model to $Z_1, \ldots, Z_M$ will lead to better results than fitting a least squares model to $X_1, \ldots, X_p$, since most or all of the information in the data that relates to the response is contained in $Z_1, \ldots, Z_M$, and by estimating only $M \ll p$ coefficients we can mitigate overfitting. In the advertising data, the first principal component explains most of the variance in both pop and ad, so a principal component regression that uses this single variable to predict some response of interest, such as sales, will likely perform quite well.

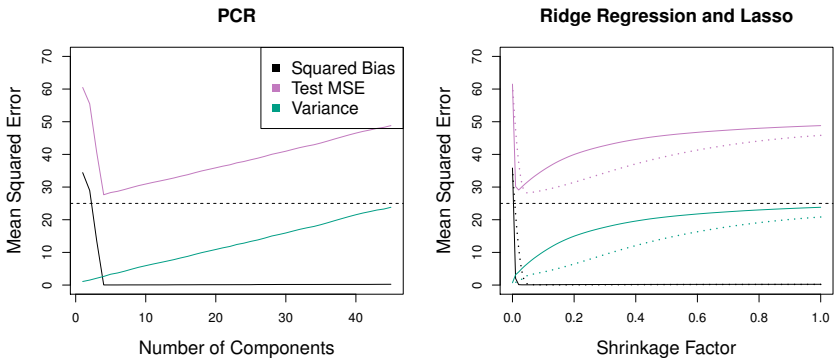


FIGURE 6.19. *PCR, ridge regression, and the lasso were applied to a simulated data set in which the first five principal components of X contain all the information about the response Y. In each panel, the irreducible error* $\mathrm{Var}(\epsilon)$ *is shown as a horizontal dashed line.* Left: *Results for PCR.* Right: *Results for lasso (solid) and ridge regression (dotted). The x-axis displays the shrinkage factor of the coefficient estimates, defined as the ℓ_2 norm of the shrunken coefficient estimates divided by the ℓ_2 norm of the least squares estimate.*

Figure 6.18 displays the PCR fits on the simulated data sets from Figures 6.8 and 6.9. Recall that both data sets were generated using $n = 50$ observations and $p = 45$ predictors. However, while the response in the first data set was a function of all the predictors, the response in the second data set was generated using only two of the predictors. The curves are plotted as a function of M, the number of principal components used as predictors in the regression model. As more principal components are used in the regression model, the bias decreases, but the variance increases. This results in a typical U-shape for the mean squared error. When $M = p = 45$, then PCR amounts simply to a least squares fit using all of the original predictors. The figure indicates that performing PCR with an appropriate choice of M can result in a substantial improvement over least squares, especially in the left-hand panel. However, by examining the ridge regression and lasso results in Figures 6.5, 6.8, and 6.9, we see that PCR does not perform as well as the two shrinkage methods in this example.

The relatively worse performance of PCR in Figure 6.18 is a consequence of the fact that the data were generated in such a way that many principal components are required in order to adequately model the response. In contrast, PCR will tend to do well in cases when the first few principal components are sufficient to capture most of the variation in the predictors as well as the relationship with the response. The left-hand panel of Figure 6.19 illustrates the results from another simulated data set designed to be more favorable to PCR. Here the response was generated in such a way that it depends exclusively on the first five principal components. Now the

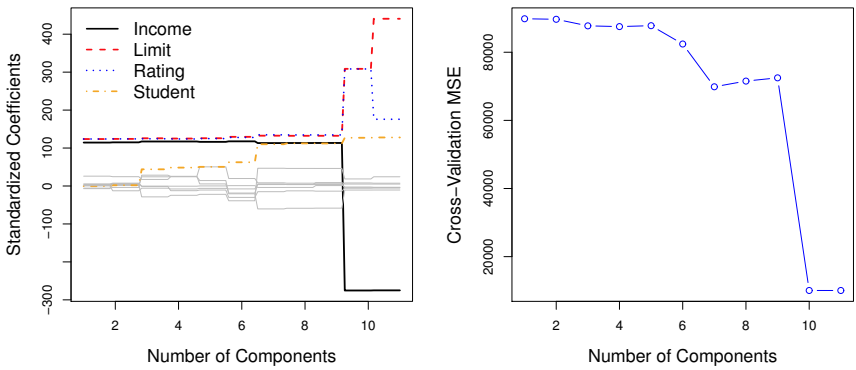


FIGURE 6.20. Left: *PCR standardized coefficient estimates on the* `Credit` *data set for different values of* M. Right: *The ten-fold cross-validation* MSE *obtained using PCR, as a function of* M.

bias drops to zero rapidly as M, the number of principal components used in PCR, increases. The mean squared error displays a clear minimum at $M = 5$. The right-hand panel of Figure 6.19 displays the results on these data using ridge regression and the lasso. All three methods offer a significant improvement over least squares. However, PCR and ridge regression slightly outperform the lasso.

We note that even though PCR provides a simple way to perform regression using $M < p$ predictors, it is *not* a feature selection method. This is because each of the M principal components used in the regression is a linear combination of all p of the *original* features. For instance, in (6.19), Z_1 was a linear combination of both `pop` and `ad`. Therefore, while PCR often performs quite well in many practical settings, it does not result in the development of a model that relies upon a small set of the original features. In this sense, PCR is more closely related to ridge regression than to the lasso. In fact, one can show that PCR and ridge regression are very closely related. One can even think of ridge regression as a continuous version of PCR![8]

In PCR, the number of principal components, M, is typically chosen by cross-validation. The results of applying PCR to the `Credit` data set are shown in Figure 6.20; the right-hand panel displays the cross-validation errors obtained, as a function of M. On these data, the lowest cross-validation error occurs when there are $M = 10$ components; this corresponds to almost no dimension reduction at all, since PCR with $M = 11$ is equivalent to simply performing least squares.

[8]More details can be found in Section 3.5 of *The Elements of Statistical Learning* by Hastie, Tibshirani, and Friedman.

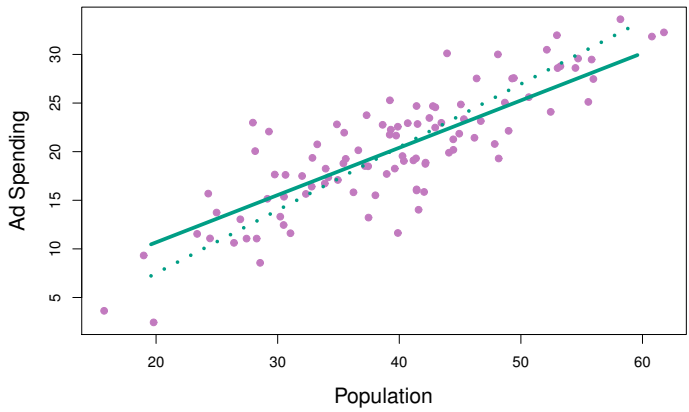


FIGURE 6.21. *For the advertising data, the first PLS direction (solid line) and first PCR direction (dotted line) are shown.*

When performing PCR, we generally recommend *standardizing* each predictor, using (6.6), prior to generating the principal components. This standardization ensures that all variables are on the same scale. In the absence of standardization, the high-variance variables will tend to play a larger role in the principal components obtained, and the scale on which the variables are measured will ultimately have an effect on the final PCR model. However, if the variables are all measured in the same units (say, kilograms, or inches), then one might choose not to standardize them.

6.3.2 Partial Least Squares

The PCR approach that we just described involves identifying linear combinations, or *directions*, that best represent the predictors $X_1, \ldots, X_p$. These directions are identified in an *unsupervised* way, since the response Y is not used to help determine the principal component directions. That is, the response does not *supervise* the identification of the principal components. Consequently, PCR suffers from a drawback: there is no guarantee that the directions that best explain the predictors will also be the best directions to use for predicting the response. Unsupervised methods are discussed further in Chapter 12.

We now present *partial least squares* (PLS), a *supervised* alternative to PCR. Like PCR, PLS is a dimension reduction method, which first identifies a new set of features $Z_1, \ldots, Z_M$ that are linear combinations of the original features, and then fits a linear model via least squares using these M new features. But unlike PCR, PLS identifies these new features in a supervised way—that is, it makes use of the response Y in order to identify new features that not only approximate the old features well, but also that *are*

partial least squares

related to the response. Roughly speaking, the PLS approach attempts to find directions that help explain both the response and the predictors.

We now describe how the first PLS direction is computed. After standardizing the p predictors, PLS computes the first direction Z_1 by setting each ϕ_{j1} in (6.16) equal to the coefficient from the simple linear regression of Y onto X_j. One can show that this coefficient is proportional to the correlation between Y and X_j. Hence, in computing $Z_1 = \sum_{j=1}^{p} \phi_{j1} X_j$, PLS places the highest weight on the variables that are most strongly related to the response.

Figure 6.21 displays an example of PLS on a synthetic dataset with Sales in each of 100 regions as the response, and two predictors; Population Size and Advertising Spending. The solid green line indicates the first PLS direction, while the dotted line shows the first principal component direction. PLS has chosen a direction that has less change in the `ad` dimension per unit change in the `pop` dimension, relative to PCA. This suggests that `pop` is more highly correlated with the response than is `ad`. The PLS direction does not fit the predictors as closely as does PCA, but it does a better job explaining the response.

To identify the second PLS direction we first *adjust* each of the variables for Z_1, by regressing each variable on Z_1 and taking *residuals*. These residuals can be interpreted as the remaining information that has not been explained by the first PLS direction. We then compute Z_2 using this *orthogonalized* data in exactly the same fashion as Z_1 was computed based on the original data. This iterative approach can be repeated M times to identify multiple PLS components $Z_1, \ldots, Z_M$. Finally, at the end of this procedure, we use least squares to fit a linear model to predict Y using $Z_1, \ldots, Z_M$ in exactly the same fashion as for PCR.

As with PCR, the number M of partial least squares directions used in PLS is a tuning parameter that is typically chosen by cross-validation. We generally standardize the predictors and response before performing PLS.

PLS is popular in the field of chemometrics, where many variables arise from digitized spectrometry signals. In practice it often performs no better than ridge regression or PCR. While the supervised dimension reduction of PLS can reduce bias, it also has the potential to increase variance, so that the overall benefit of PLS relative to PCR is a wash.

6.4 Considerations in High Dimensions

6.4.1 High-Dimensional Data

Most traditional statistical techniques for regression and classification are intended for the *low-dimensional* setting in which n, the number of observations, is much greater than p, the number of features. This is due in part to the fact that throughout most of the field's history, the bulk of sci-

low-dimensional

entific problems requiring the use of statistics have been low-dimensional. For instance, consider the task of developing a model to predict a patient's blood pressure on the basis of his or her age, sex, and body mass index (BMI). There are three predictors, or four if an intercept is included in the model, and perhaps several thousand patients for whom blood pressure and age, sex, and BMI are available. Hence $n \gg p$, and so the problem is low-dimensional. (By dimension here we are referring to the size of p.)

In the past 20 years, new technologies have changed the way that data are collected in fields as diverse as finance, marketing, and medicine. It is now commonplace to collect an almost unlimited number of feature measurements (p very large). While p can be extremely large, the number of observations n is often limited due to cost, sample availability, or other considerations. Two examples are as follows:

1. Rather than predicting blood pressure on the basis of just age, sex, and BMI, one might also collect measurements for half a million *single nucleotide polymorphisms* (SNPs; these are individual DNA mutations that are relatively common in the population) for inclusion in the predictive model. Then $n \approx 200$ and $p \approx 500{,}000$.

2. A marketing analyst interested in understanding people's online shopping patterns could treat as features all of the search terms entered by users of a search engine. This is sometimes known as the "bag-of-words" model. The same researcher might have access to the search histories of only a few hundred or a few thousand search engine users who have consented to share their information with the researcher. For a given user, each of the p search terms is scored present (0) or absent (1), creating a large binary feature vector. Then $n \approx 1{,}000$ and p is much larger.

Data sets containing more features than observations are often referred to as *high-dimensional*. Classical approaches such as least squares linear regression are not appropriate in this setting. Many of the issues that arise in the analysis of high-dimensional data were discussed earlier in this book, since they apply also when $n > p$: these include the role of the bias-variance trade-off and the danger of overfitting. Though these issues are always relevant, they can become particularly important when the number of features is very large relative to the number of observations.

high-dimensional

We have defined the *high-dimensional setting* as the case where the number of features p is larger than the number of observations n. But the considerations that we will now discuss certainly also apply if p is slightly smaller than n, and are best always kept in mind when performing supervised learning.

6.4.2 What Goes Wrong in High Dimensions?

In order to illustrate the need for extra care and specialized techniques for regression and classification when $p > n$, we begin by examining what can go wrong if we apply a statistical technique not intended for the high-dimensional setting. For this purpose, we examine least squares regression. But the same concepts apply to logistic regression, linear discriminant analysis, and other classical statistical approaches.

When the number of features p is as large as, or larger than, the number of observations n, least squares as described in Chapter 3 cannot (or rather, *should not*) be performed. The reason is simple: regardless of whether or not there truly is a relationship between the features and the response, least squares will yield a set of coefficient estimates that result in a perfect fit to the data, such that the residuals are zero.

An example is shown in Figure 6.22 with $p = 1$ feature (plus an intercept) in two cases: when there are 20 observations, and when there are only two observations. When there are 20 observations, $n > p$ and the least squares regression line does not perfectly fit the data; instead, the regression line seeks to approximate the 20 observations as well as possible. On the other hand, when there are only two observations, then regardless of the values of those observations, the regression line will fit the data exactly. This is problematic because this perfect fit will almost certainly lead to overfitting of the data. In other words, though it is possible to perfectly fit the training data in the high-dimensional setting, the resulting linear model will perform extremely poorly on an independent test set, and therefore does not constitute a useful model. In fact, we can see that this happened in Figure 6.22: the least squares line obtained in the right-hand panel will perform very poorly on a test set comprised of the observations in the left-hand panel. The problem is simple: when $p > n$ or $p \approx n$, a simple least squares regression line is too *flexible* and hence overfits the data.

Figure 6.23 further illustrates the risk of carelessly applying least squares when the number of features p is large. Data were simulated with $n = 20$ observations, and regression was performed with between 1 and 20 features, each of which was completely unrelated to the response. As shown in the figure, the model R^2 increases to 1 as the number of features included in the model increases, and correspondingly the training set MSE decreases to 0 as the number of features increases, *even though the features are completely unrelated to the response*. On the other hand, the MSE on an *independent test set* becomes extremely large as the number of features included in the model increases, because including the additional predictors leads to a vast increase in the variance of the coefficient estimates. Looking at the test set MSE, it is clear that the best model contains at most a few variables. However, someone who carelessly examines only the R^2 or the training set MSE might erroneously conclude that the model with the greatest number of variables is best. This indicates the importance of applying extra care

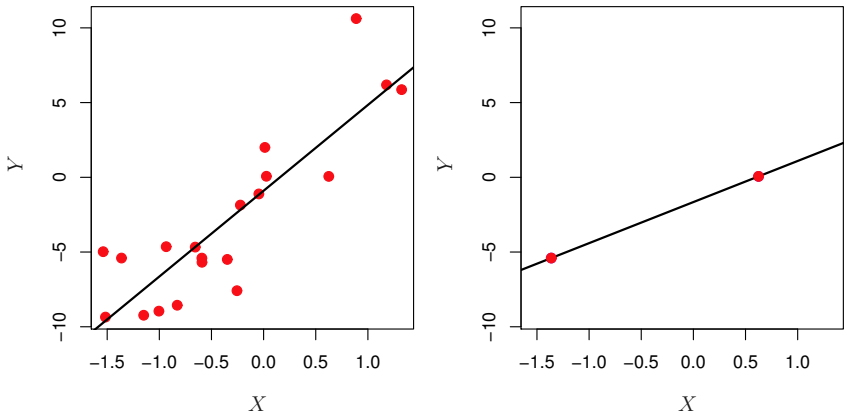


FIGURE 6.22. Left: *Least squares regression in the low-dimensional setting.* Right: *Least squares regression with* $n = 2$ *observations and two parameters to be estimated (an intercept and a coefficient).*

when analyzing data sets with a large number of variables, and of always evaluating model performance on an independent test set.

In Section 6.1.3, we saw a number of approaches for adjusting the training set RSS or R^2 in order to account for the number of variables used to fit a least squares model. Unfortunately, the C_p, AIC, and BIC approaches are not appropriate in the high-dimensional setting, because estimating $\hat{\sigma}^2$ is problematic. (For instance, the formula for $\hat{\sigma}^2$ from Chapter 3 yields an estimate $\hat{\sigma}^2 = 0$ in this setting.) Similarly, problems arise in the application of adjusted R^2 in the high-dimensional setting, since one can easily obtain a model with an adjusted R^2 value of 1. Clearly, alternative approaches that are better-suited to the high-dimensional setting are required.

6.4.3 Regression in High Dimensions

It turns out that many of the methods seen in this chapter for fitting *less flexible* least squares models, such as forward stepwise selection, ridge regression, the lasso, and principal components regression, are particularly useful for performing regression in the high-dimensional setting. Essentially, these approaches avoid overfitting by using a less flexible fitting approach than least squares.

Figure 6.24 illustrates the performance of the lasso in a simple simulated example. There are $p = 20$, 50, or 2,000 features, of which 20 are truly associated with the outcome. The lasso was performed on $n = 100$ training observations, and the mean squared error was evaluated on an independent test set. As the number of features increases, the test set error increases. When $p = 20$, the lowest validation set error was achieved when λ in (6.7) was small; however, when p was larger then the lowest validation

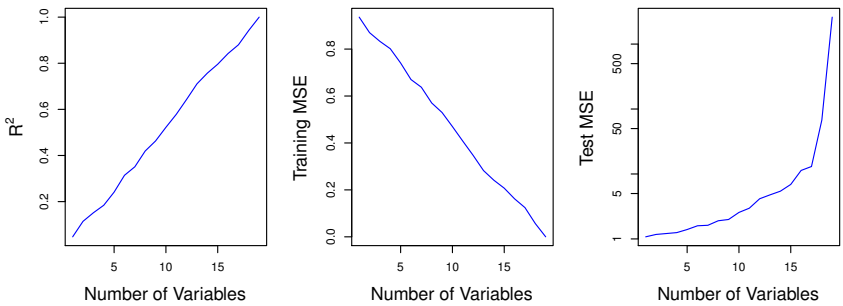


FIGURE 6.23. *On a simulated example with $n = 20$ training observations, features that are completely unrelated to the outcome are added to the model.* Left: *The R^2 increases to 1 as more features are included.* Center: *The training set MSE decreases to 0 as more features are included.* Right: *The test set MSE increases as more features are included.*

set error was achieved using a larger value of λ. In each boxplot, rather than reporting the values of λ used, the *degrees of freedom* of the resulting lasso solution is displayed; this is simply the number of non-zero coefficient estimates in the lasso solution, and is a measure of the flexibility of the lasso fit. Figure 6.24 highlights three important points: (1) regularization or shrinkage plays a key role in high-dimensional problems, (2) appropriate tuning parameter selection is crucial for good predictive performance, and (3) the test error tends to increase as the dimensionality of the problem (i.e. the number of features or predictors) increases, unless the additional features are truly associated with the response.

curse of dimensionality

The third point above is in fact a key principle in the analysis of high-dimensional data, which is known as the *curse of dimensionality*. One might think that as the number of features used to fit a model increases, the quality of the fitted model will increase as well. However, comparing the left-hand and right-hand panels in Figure 6.24, we see that this is not necessarily the case: in this example, the test set MSE almost doubles as p increases from 20 to 2,000. In general, *adding additional signal features that are truly associated with the response will improve the fitted model*, in the sense of leading to a reduction in test set error. However, adding noise features that are not truly associated with the response will lead to a deterioration in the fitted model, and consequently an increased test set error. This is because noise features increase the dimensionality of the problem, exacerbating the risk of overfitting (since noise features may be assigned nonzero coefficients due to chance associations with the response on the training set) without any potential upside in terms of improved test set error. Thus, we see that new technologies that allow for the collection of measurements for thousands or millions of features are a double-edged sword: they can lead to improved predictive models if these features are in

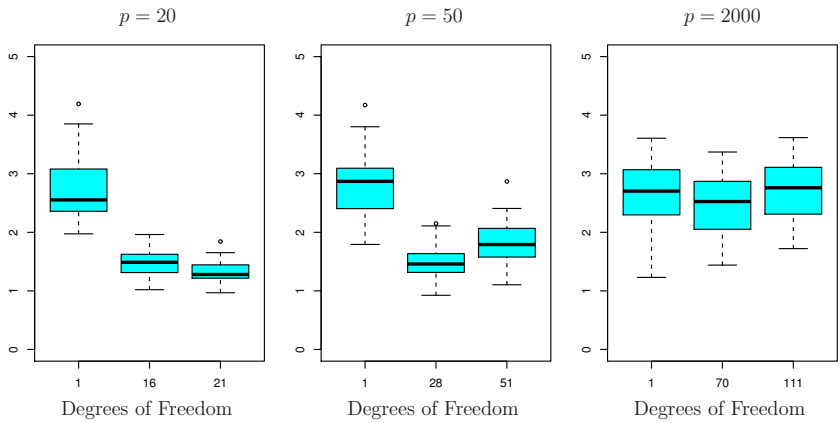


FIGURE 6.24. *The lasso was performed with* $n = 100$ *observations and three values of* p*, the number of features. Of the* p *features, 20 were associated with the response. The boxplots show the test MSEs that result using three different values of the tuning parameter* λ *in (6.7). For ease of interpretation, rather than reporting* λ*, the* degrees of freedom *are reported; for the lasso this turns out to be simply the number of estimated non-zero coefficients. When* $p = 20$*, the lowest test MSE was obtained with the smallest amount of regularization. When* $p = 50$*, the lowest test MSE was achieved when there is a substantial amount of regularization. When* $p = 2{,}000$ *the lasso performed poorly regardless of the amount of regularization, due to the fact that only 20 of the 2,000 features truly are associated with the outcome.*

fact relevant to the problem at hand, but will lead to worse results if the features are not relevant. Even if they are relevant, the variance incurred in fitting their coefficients may outweigh the reduction in bias that they bring.

6.4.4 Interpreting Results in High Dimensions

When we perform the lasso, ridge regression, or other regression procedures in the high-dimensional setting, we must be quite cautious in the way that we report the results obtained. In Chapter 3, we learned about *multicollinearity*, the concept that the variables in a regression might be correlated with each other. In the high-dimensional setting, the multicollinearity problem is extreme: any variable in the model can be written as a linear combination of all of the other variables in the model. Essentially, this means that we can never know exactly which variables (if any) truly are predictive of the outcome, and we can never identify the *best* coefficients for use in the regression. At most, we can hope to assign large regression coefficients to variables that are correlated with the variables that truly are predictive of the outcome.

For instance, suppose that we are trying to predict blood pressure on the basis of half a million SNPs, and that forward stepwise selection indicates that 17 of those SNPs lead to a good predictive model on the training data. It would be incorrect to conclude that these 17 SNPs predict blood pressure more effectively than the other SNPs not included in the model. There are likely to be many sets of 17 SNPs that would predict blood pressure just as well as the selected model. If we were to obtain an independent data set and perform forward stepwise selection on that data set, we would likely obtain a model containing a different, and perhaps even non-overlapping, set of SNPs. This does not detract from the value of the model obtained—for instance, the model might turn out to be very effective in predicting blood pressure on an independent set of patients, and might be clinically useful for physicians. But we must be careful not to overstate the results obtained, and to make it clear that what we have identified is simply *one of many possible models* for predicting blood pressure, and that it must be further validated on independent data sets.

It is also important to be particularly careful in reporting errors and measures of model fit in the high-dimensional setting. We have seen that when $p > n$, it is easy to obtain a useless model that has zero residuals. Therefore, one should *never* use sum of squared errors, p-values, R^2 statistics, or other traditional measures of model fit on the training data as evidence of a good model fit in the high-dimensional setting. For instance, as we saw in Figure 6.23, one can easily obtain a model with $R^2 = 1$ when $p > n$. Reporting this fact might mislead others into thinking that a statistically valid and useful model has been obtained, whereas in fact this provides absolutely no evidence of a compelling model. It is important to instead report results on an independent test set, or cross-validation errors. For instance, the MSE or R^2 on an independent test set is a valid measure of model fit, but the MSE on the training set certainly is not.

6.5 Lab: Linear Models and Regularization Methods

6.5.1 Subset Selection Methods

Best Subset Selection

Here we apply the best subset selection approach to the `Hitters` data. We wish to predict a baseball player's `Salary` on the basis of various statistics associated with performance in the previous year.

First of all, we note that the `Salary` variable is missing for some of the players. The `is.na()` function can be used to identify the missing observations. It returns a vector of the same length as the input vector, with a `TRUE` `is.na()`

for any elements that are missing, and a FALSE for non-missing elements. The sum() function can then be used to count all of the missing elements.

sum()

```
> library(ISLR2)
> View(Hitters)
> names(Hitters)
 [1] "AtBat"     "Hits"      "HmRun"     "Runs"      "RBI"
 [6] "Walks"     "Years"     "CAtBat"    "CHits"     "CHmRun"
[11] "CRuns"     "CRBI"      "CWalks"    "League"    "Division"
[16] "PutOuts"   "Assists"   "Errors"    "Salary"    "NewLeague"
> dim(Hitters)
[1] 322  20
> sum(is.na(Hitters$Salary))
[1] 59
```

Hence we see that Salary is missing for 59 players. The na.omit() function removes all of the rows that have missing values in any variable.

```
> Hitters <- na.omit(Hitters)
> dim(Hitters)
[1] 263  20
> sum(is.na(Hitters))
[1] 0
```

The regsubsets() function (part of the leaps library) performs best subset selection by identifying the best model that contains a given number of predictors, where *best* is quantified using RSS. The syntax is the same as for lm(). The summary() command outputs the best set of variables for each model size.

regsubsets()

```
> library(leaps)
> regfit.full <- regsubsets(Salary ~ ., Hitters)
> summary(regfit.full)
Subset selection object
Call: regsubsets.formula(Salary ~ ., Hitters)
19 Variables  (and intercept)
...
1 subsets of each size up to 8
Selection Algorithm: exhaustive
         AtBat Hits HmRun Runs RBI Walks Years CAtBat CHits
1  ( 1 ) " "   " "  " "   " "  " " " "   " "   " "    " "
2  ( 1 ) " "   "*"  " "   " "  " " " "   " "   " "    " "
3  ( 1 ) " "   "*"  " "   " "  " " " "   " "   " "    " "
4  ( 1 ) " "   "*"  " "   " "  " " " "   " "   " "    " "
5  ( 1 ) "*"   "*"  " "   " "  " " " "   " "   " "    " "
6  ( 1 ) "*"   "*"  " "   " "  " " " "   " "   " "    " "
7  ( 1 ) " "   "*"  " "   " "  " " " "   " "   "*"    "*"
8  ( 1 ) "*"   "*"  " "   " "  " " " "   " "   " "    " "
         CHmRun CRuns CRBI CWalks LeagueN DivisionW PutOuts
1  ( 1 ) " "    " "   "*"  " "    " "     " "       " "
2  ( 1 ) " "    " "   "*"  " "    " "     " "       " "
3  ( 1 ) " "    " "   "*"  " "    " "     " "       "*"
4  ( 1 ) " "    " "   "*"  " "    " "     "*"       "*"
5  ( 1 ) " "    " "   "*"  " "    " "     "*"       "*"
```

```
6  ( 1 ) " "     " "    "*"   " "     " "      "*"        "*"
7  ( 1 ) "*"     " "    " "   " "     " "      "*"        "*"
8  ( 1 ) "*"     "*"    " "   "*"     " "      "*"        "*"
          Assists Errors NewLeagueN
1  ( 1 ) " "     " "    " "
2  ( 1 ) " "     " "    " "
3  ( 1 ) " "     " "    " "
4  ( 1 ) " "     " "    " "
5  ( 1 ) " "     " "    " "
6  ( 1 ) " "     " "    " "
7  ( 1 ) " "     " "    " "
8  ( 1 ) " "     " "    " "
```

An asterisk indicates that a given variable is included in the corresponding model. For instance, this output indicates that the best two-variable model contains only `Hits` and `CRBI`. By default, `regsubsets()` only reports results up to the best eight-variable model. But the `nvmax` option can be used in order to return as many variables as are desired. Here we fit up to a 19-variable model.

```
> regfit.full <- regsubsets(Salary ~ ., data = Hitters,
    nvmax = 19)
> reg.summary <- summary(regfit.full)
```

The `summary()` function also returns R^2, RSS, adjusted R^2, C_p, and BIC. We can examine these to try to select the *best* overall model.

```
> names(reg.summary)
[1] "which"  "rsq"    "rss"    "adjr2"  "cp"     "bic"
[7] "outmat" "obj"
```

For instance, we see that the R^2 statistic increases from 32 %, when only one variable is included in the model, to almost 55 %, when all variables are included. As expected, the R^2 statistic increases monotonically as more variables are included.

```
> reg.summary$rsq
 [1] 0.321 0.425 0.451 0.475 0.491 0.509 0.514 0.529 0.535
[10] 0.540 0.543 0.544 0.544 0.545 0.545 0.546 0.546 0.546
[19] 0.546
```

Plotting RSS, adjusted R^2, C_p, and BIC for all of the models at once will help us decide which model to select. Note the `type = "l"` option tells `R` to connect the plotted points with lines.

```
> par(mfrow = c(2, 2))
> plot(reg.summary$rss, xlab = "Number of Variables",
    ylab = "RSS", type = "l")
> plot(reg.summary$adjr2, xlab = "Number of Variables",
    ylab = "Adjusted RSq", type = "l")
```

The `points()` command works like the `plot()` command, except that it puts points on a plot that has already been created, instead of creating a new plot. The `which.max()` function can be used to identify the location of

`points()`

the maximum point of a vector. We will now plot a red dot to indicate the model with the largest adjusted R^2 statistic.

```
> which.max(reg.summary$adjr2)
[1] 11
> points(11, reg.summary$adjr2[11], col = "red", cex = 2,
    pch = 20)
```

In a similar fashion we can plot the C_p and BIC statistics, and indicate the models with the smallest statistic using `which.min()`.

`which.min()`

```
> plot(reg.summary$cp, xlab = "Number of Variables",
    ylab = "Cp", type = "l")
> which.min(reg.summary$cp)
[1] 10
> points(10, reg.summary$cp[10], col = "red", cex = 2,
    pch = 20)
> which.min(reg.summary$bic)
[1] 6
> plot(reg.summary$bic, xlab = "Number of Variables",
    ylab = "BIC", type = "l")
> points(6, reg.summary$bic[6], col = "red", cex = 2,
    pch = 20)
```

The `regsubsets()` function has a built-in `plot()` command which can be used to display the selected variables for the best model with a given number of predictors, ranked according to the BIC, C_p, adjusted R^2, or AIC. To find out more about this function, type `?plot.regsubsets`.

```
> plot(regfit.full, scale = "r2")
> plot(regfit.full, scale = "adjr2")
> plot(regfit.full, scale = "Cp")
> plot(regfit.full, scale = "bic")
```

The top row of each plot contains a black square for each variable selected according to the optimal model associated with that statistic. For instance, we see that several models share a BIC close to −150. However, the model with the lowest BIC is the six-variable model that contains only `AtBat`, `Hits`, `Walks`, `CRBI`, `DivisionW`, and `PutOuts`. We can use the `coef()` function to see the coefficient estimates associated with this model.

```
> coef(regfit.full, 6)
(Intercept)       AtBat        Hits       Walks        CRBI
     91.512      -1.869       7.604       3.698       0.643
  DivisionW     PutOuts
   -122.952       0.264
```

Forward and Backward Stepwise Selection

We can also use the `regsubsets()` function to perform forward stepwise or backward stepwise selection, using the argument `method = "forward"` or `method = "backward"`.

```
> regfit.fwd <- regsubsets(Salary ~ ., data = Hitters,
    nvmax = 19, method = "forward")
> summary(regfit.fwd)
> regfit.bwd <- regsubsets(Salary ~ ., data = Hitters,
    nvmax = 19, method = "backward")
> summary(regfit.bwd)
```

For instance, we see that using forward stepwise selection, the best one-variable model contains only `CRBI`, and the best two-variable model additionally includes `Hits`. For this data, the best one-variable through six-variable models are each identical for best subset and forward selection. However, the best seven-variable models identified by forward stepwise selection, backward stepwise selection, and best subset selection are different.

```
> coef(regfit.full, 7)
(Intercept)        Hits       Walks      CAtBat       CHits
     79.451       1.283       3.227      -0.375       1.496
    CHmRun   DivisionW     PutOuts
      1.442    -129.987       0.237
> coef(regfit.fwd, 7)
(Intercept)       AtBat        Hits       Walks        CRBI
    109.787      -1.959       7.450       4.913       0.854
     CWalks   DivisionW     PutOuts
     -0.305    -127.122       0.253
> coef(regfit.bwd, 7)
(Intercept)       AtBat        Hits       Walks       CRuns
    105.649      -1.976       6.757       6.056       1.129
     CWalks   DivisionW     PutOuts
     -0.716    -116.169       0.303
```

Choosing Among Models Using the Validation-Set Approach and Cross-Validation

We just saw that it is possible to choose among a set of models of different sizes using C_p, BIC, and adjusted R^2. We will now consider how to do this using the validation set and cross-validation approaches.

In order for these approaches to yield accurate estimates of the test error, we must use *only the training observations* to perform all aspects of model-fitting—including variable selection. Therefore, the determination of which model of a given size is best must be made using *only the training observations*. This point is subtle but important. If the full data set is used to perform the best subset selection step, the validation set errors and cross-validation errors that we obtain will not be accurate estimates of the test error.

In order to use the validation set approach, we begin by splitting the observations into a training set and a test set. We do this by creating a random vector, `train`, of elements equal to `TRUE` if the corresponding observation is in the training set, and `FALSE` otherwise. The vector `test` has a `TRUE` if the observation is in the test set, and a `FALSE` otherwise. Note the

! in the command to create test causes TRUEs to be switched to FALSEs and vice versa. We also set a random seed so that the user will obtain the same training set/test set split.

```
> set.seed(1)
> train <- sample(c(TRUE, FALSE), nrow(Hitters),
    replace = TRUE)
> test <- (!train)
```

Now, we apply regsubsets() to the training set in order to perform best subset selection.

```
> regfit.best <- regsubsets(Salary ~ .,
    data = Hitters[train, ], nvmax = 19)
```

Notice that we subset the Hitters data frame directly in the call in order to access only the training subset of the data, using the expression Hitters[train,]. We now compute the validation set error for the best model of each model size. We first make a model matrix from the test data.

```
> test.mat <- model.matrix(Salary ~ ., data = Hitters[test, ])
```

The model.matrix() function is used in many regression packages for building an "X" matrix from data. Now we run a loop, and for each size i, we extract the coefficients from regfit.best for the best model of that size, multiply them into the appropriate columns of the test model matrix to form the predictions, and compute the test MSE.

model.matrix()

```
> val.errors <- rep(NA, 19)
> for (i in 1:19) {
+  coefi <- coef(regfit.best, id = i)
+  pred <- test.mat[, names(coefi)] %*% coefi
+  val.errors[i] <- mean((Hitters$Salary[test] - pred)^2)
}
```

We find that the best model is the one that contains seven variables.

```
> val.errors
 [1] 164377 144405 152176 145198 137902 139176 126849 136191
 [9] 132890 135435 136963 140695 140691 141951 141508 142164
[17] 141767 142340 142238
> which.min(val.errors)
[1] 7
> coef(regfit.best, 7)
(Intercept)       AtBat        Hits       Walks       CRuns
     67.109      -2.146       7.015       8.072       1.243
     CWalks   DivisionW     PutOuts
     -0.834    -118.436       0.253
```

This was a little tedious, partly because there is no predict() method for regsubsets(). Since we will be using this function again, we can capture our steps above and write our own predict method.

```
> predict.regsubsets <- function(object, newdata, id, ...) {
+   form <- as.formula(object$call[[2]])
+   mat <- model.matrix(form, newdata)
+   coefi <- coef(object, id = id)
+   xvars <- names(coefi)
+   mat[, xvars] %*% coefi
+ }
```

Our function pretty much mimics what we did above. The only complex part is how we extracted the formula used in the call to `regsubsets()`. We demonstrate how we use this function below, when we do cross-validation.

Finally, we perform best subset selection on the full data set, and select the best seven-variable model. It is important that we make use of the full data set in order to obtain more accurate coefficient estimates. Note that we perform best subset selection on the full data set and select the best seven-variable model, rather than simply using the variables that were obtained from the training set, because the best seven-variable model on the full data set may differ from the corresponding model on the training set.

```
> regfit.best <- regsubsets(Salary ~ ., data = Hitters,
    nvmax = 19)
> coef(regfit.best, 7)
(Intercept)        Hits       Walks      CAtBat       CHits
     79.451       1.283       3.227      -0.375       1.496
     CHmRun   DivisionW     PutOuts
      1.442    -129.987       0.237
```

In fact, we see that the best seven-variable model on the full data set has a different set of variables than the best seven-variable model on the training set.

We now try to choose among the models of different sizes using cross-validation. This approach is somewhat involved, as we must perform best subset selection *within each of the k training sets*. Despite this, we see that with its clever subsetting syntax, `R` makes this job quite easy. First, we create a vector that allocates each observation to one of $k = 10$ folds, and we create a matrix in which we will store the results.

```
> k <- 10
> n <- nrow(Hitters)
> set.seed(1)
> folds <- sample(rep(1:k, length = n))
> cv.errors <- matrix(NA, k, 19,
    dimnames = list(NULL, paste(1:19)))
```

Now we write a for loop that performs cross-validation. In the jth fold, the elements of `folds` that equal `j` are in the test set, and the remainder are in the training set. We make our predictions for each model size (using our new `predict()` method), compute the test errors on the appropriate subset, and store them in the appropriate slot in the matrix `cv.errors`. Note that in the

following code R will automatically use our `predict.regsubsets()` function when we call `predict()` because the `best.fit` object has class `regsubsets`.

```
> for (j in 1:k) {
+   best.fit <- regsubsets(Salary ~ .,
       data = Hitters[folds != j, ],
       nvmax = 19)
+   for (i in 1:19) {
+     pred <- predict(best.fit, Hitters[folds == j, ], id = i)
+     cv.errors[j, i] <-
         mean((Hitters$Salary[folds == j] - pred)^2)
+    }
+  }
```

This has given us a 10×19 matrix, of which the (j, i)th element corresponds to the test MSE for the jth cross-validation fold for the best i-variable model. We use the `apply()` function to average over the columns of this matrix in order to obtain a vector for which the ith element is the cross-validation error for the i-variable model.

`apply()`

```
> mean.cv.errors <- apply(cv.errors, 2, mean)
> mean.cv.errors
     1      2      3      4      5      6      7      8
143440 126817 134214 131783 130766 120383 121443 114364
     9     10     11     12     13     14     15     16
115163 109366 112738 113617 115558 115853 115631 116050
    17     18     19
116117 116419 116299
> par(mfrow = c(1, 1))
> plot(mean.cv.errors, type = "b")
```

We see that cross-validation selects a 10-variable model. We now perform best subset selection on the full data set in order to obtain the 10-variable model.

```
> reg.best <- regsubsets(Salary ~ ., data = Hitters,
    nvmax = 19)
> coef(reg.best, 10)
(Intercept)       AtBat        Hits       Walks      CAtBat
    162.535      -2.169       6.918       5.773      -0.130
      CRuns        CRBI      CWalks   DivisionW     PutOuts
      1.408       0.774      -0.831    -112.380       0.297
    Assists
      0.283
```

6.5.2 *Ridge Regression and the Lasso*

We will use the `glmnet` package in order to perform ridge regression and the lasso. The main function in this package is `glmnet()`, which can be used to fit ridge regression models, lasso models, and more. This function has slightly different syntax from other model-fitting functions that we have encountered thus far in this book. In particular, we must pass in an `x`

`glmnet()`

matrix as well as a `y` vector, and we do not use the `y ~ x` syntax. We will now perform ridge regression and the lasso in order to predict `Salary` on the `Hitters` data. Before proceeding ensure that the missing values have been removed from the data, as described in Section 6.5.1.

```
> x <- model.matrix(Salary ~ ., Hitters)[, -1]
> y <- Hitters$Salary
```

The `model.matrix()` function is particularly useful for creating `x`; not only does it produce a matrix corresponding to the 19 predictors but it also automatically transforms any qualitative variables into dummy variables. The latter property is important because `glmnet()` can only take numerical, quantitative inputs.

Ridge Regression

The `glmnet()` function has an `alpha` argument that determines what type of model is fit. If `alpha=0` then a ridge regression model is fit, and if `alpha=1` then a lasso model is fit. We first fit a ridge regression model.

```
> library(glmnet)
> grid <- 10^seq(10, -2, length = 100)
> ridge.mod <- glmnet(x, y, alpha = 0, lambda = grid)
```

By default the `glmnet()` function performs ridge regression for an automatically selected range of λ values. However, here we have chosen to implement the function over a grid of values ranging from $\lambda = 10^{10}$ to $\lambda = 10^{-2}$, essentially covering the full range of scenarios from the null model containing only the intercept, to the least squares fit. As we will see, we can also compute model fits for a particular value of λ that is not one of the original `grid` values. Note that by default, the `glmnet()` function standardizes the variables so that they are on the same scale. To turn off this default setting, use the argument `standardize = FALSE`.

Associated with each value of λ is a vector of ridge regression coefficients, stored in a matrix that can be accessed by `coef()`. In this case, it is a 20×100 matrix, with 20 rows (one for each predictor, plus an intercept) and 100 columns (one for each value of λ).

```
> dim(coef(ridge.mod))
[1]  20 100
```

We expect the coefficient estimates to be much smaller, in terms of ℓ_2 norm, when a large value of λ is used, as compared to when a small value of λ is used. These are the coefficients when $\lambda = 11{,}498$, along with their ℓ_2 norm:

```
> ridge.mod$lambda[50]
[1] 11498
> coef(ridge.mod)[, 50]
(Intercept)       AtBat        Hits       HmRun        Runs
    407.356       0.037       0.138       0.525       0.231
        RBI       Walks       Years      CAtBat       CHits
```

```
      0.240       0.290       1.108       0.003       0.012
     CHmRun       CRuns        CRBI      CWalks     LeagueN
      0.088       0.023       0.024       0.025       0.085
  DivisionW     PutOuts     Assists      Errors  NewLeagueN
     -6.215       0.016       0.003      -0.021       0.301
> sqrt(sum(coef(ridge.mod)[-1, 50]^2))
[1] 6.36
```

In contrast, here are the coefficients when $\lambda = 705$, along with their ℓ_2 norm. Note the much larger ℓ_2 norm of the coefficients associated with this smaller value of λ.

```
> ridge.mod$lambda[60]
[1] 705
> coef(ridge.mod)[, 60]
(Intercept)       AtBat        Hits       HmRun        Runs
     54.325       0.112       0.656       1.180       0.938
        RBI       Walks       Years      CAtBat       CHits
      0.847       1.320       2.596       0.011       0.047
     CHmRun       CRuns        CRBI      CWalks     LeagueN
      0.338       0.094       0.098       0.072      13.684
  DivisionW     PutOuts     Assists      Errors  NewLeagueN
    -54.659       0.119       0.016      -0.704       8.612
> sqrt(sum(coef(ridge.mod)[-1, 60]^2))
[1] 57.1
```

We can use the `predict()` function for a number of purposes. For instance, we can obtain the ridge regression coefficients for a new value of λ, say 50:

```
> predict(ridge.mod, s = 50, type = "coefficients")[1:20, ]
(Intercept)       AtBat        Hits       HmRun        Runs
     48.766      -0.358       1.969      -1.278       1.146
        RBI       Walks       Years      CAtBat       CHits
      0.804       2.716      -6.218       0.005       0.106
     CHmRun       CRuns        CRBI      CWalks     LeagueN
      0.624       0.221       0.219      -0.150      45.926
  DivisionW     PutOuts     Assists      Errors  NewLeagueN
   -118.201       0.250       0.122      -3.279      -9.497
```

We now split the samples into a training set and a test set in order to estimate the test error of ridge regression and the lasso. There are two common ways to randomly split a data set. The first is to produce a random vector of `TRUE`, `FALSE` elements and select the observations corresponding to `TRUE` for the training data. The second is to randomly choose a subset of numbers between 1 and n; these can then be used as the indices for the training observations. The two approaches work equally well. We used the former method in Section 6.5.1. Here we demonstrate the latter approach.

We first set a random seed so that the results obtained will be reproducible.

```
> set.seed(1)
> train <- sample(1:nrow(x), nrow(x) / 2)
> test <- (-train)
> y.test <- y[test]
```

Next we fit a ridge regression model on the training set, and evaluate its MSE on the test set, using $\lambda = 4$. Note the use of the `predict()` function again. This time we get predictions for a test set, by replacing `type="coefficients"` with the `newx` argument.

```
> ridge.mod <- glmnet(x[train, ], y[train], alpha = 0,
    lambda = grid, thresh = 1e-12)
> ridge.pred <- predict(ridge.mod, s = 4, newx = x[test, ])
> mean((ridge.pred - y.test)^2)
[1] 142199
```

The test MSE is 142,199. Note that if we had instead simply fit a model with just an intercept, we would have predicted each test observation using the mean of the training observations. In that case, we could compute the test set MSE like this:

```
> mean((mean(y[train]) - y.test)^2)
[1] 224670
```

We could also get the same result by fitting a ridge regression model with a *very* large value of λ. Note that `1e10` means 10^{10}.

```
> ridge.pred <- predict(ridge.mod, s = 1e10, newx = x[test, ])
> mean((ridge.pred - y.test)^2)
[1] 224670
```

So fitting a ridge regression model with $\lambda = 4$ leads to a much lower test MSE than fitting a model with just an intercept. We now check whether there is any benefit to performing ridge regression with $\lambda = 4$ instead of just performing least squares regression. Recall that least squares is simply ridge regression with $\lambda = 0$.[9]

```
> ridge.pred <- predict(ridge.mod, s = 0, newx = x[test, ],
    exact = T, x = x[train, ], y = y[train])
> mean((ridge.pred - y.test)^2)
[1] 168589
> lm(y ~ x, subset = train)
> predict(ridge.mod, s = 0, exact = T, type = "coefficients",
    x = x[train, ], y = y[train])[1:20, ]
```

In general, if we want to fit a (unpenalized) least squares model, then we should use the `lm()` function, since that function provides more useful outputs, such as standard errors and p-values for the coefficients.

In general, instead of arbitrarily choosing $\lambda = 4$, it would be better to use cross-validation to choose the tuning parameter λ. We can do this using

[9] In order for `glmnet()` to yield the exact least squares coefficients when $\lambda = 0$, we use the argument `exact = T` when calling the `predict()` function. Otherwise, the `predict()` function will interpolate over the grid of λ values used in fitting the `glmnet()` model, yielding approximate results. When we use `exact = T`, there remains a slight discrepancy in the third decimal place between the output of `glmnet()` when $\lambda = 0$ and the output of `lm()`; this is due to numerical approximation on the part of `glmnet()`.

the built-in cross-validation function, `cv.glmnet()`. By default, the function performs ten-fold cross-validation, though this can be changed using the argument `nfolds`. Note that we set a random seed first so our results will be reproducible, since the choice of the cross-validation folds is random.

`cv.glmnet()`

```
> set.seed(1)
> cv.out <- cv.glmnet(x[train, ], y[train], alpha = 0)
> plot(cv.out)
> bestlam <- cv.out$lambda.min
> bestlam
[1] 326
```

Therefore, we see that the value of λ that results in the smallest cross-validation error is 326. What is the test MSE associated with this value of λ?

```
> ridge.pred <- predict(ridge.mod, s = bestlam,
    newx = x[test, ])
> mean((ridge.pred - y.test)^2)
[1] 139857
```

This represents a further improvement over the test MSE that we got using $\lambda = 4$. Finally, we refit our ridge regression model on the full data set, using the value of λ chosen by cross-validation, and examine the coefficient estimates.

```
> out <- glmnet(x, y, alpha = 0)
> predict(out, type = "coefficients", s = bestlam)[1:20, ]
(Intercept)        AtBat         Hits        HmRun         Runs
      15.44         0.08         0.86         0.60         1.06
        RBI        Walks        Years       CAtBat        CHits
       0.88         1.62         1.35         0.01         0.06
     CHmRun        CRuns         CRBI       CWalks     LeagueN
       0.41         0.11         0.12         0.05       22.09
  DivisionW      PutOuts      Assists       Errors   NewLeagueN
     -79.04         0.17         0.03        -1.36         9.12
```

As expected, none of the coefficients are zero—ridge regression does not perform variable selection!

The Lasso

We saw that ridge regression with a wise choice of λ can outperform least squares as well as the null model on the `Hitters` data set. We now ask whether the lasso can yield either a more accurate or a more interpretable model than ridge regression. In order to fit a lasso model, we once again use the `glmnet()` function; however, this time we use the argument `alpha=1`. Other than that change, we proceed just as we did in fitting a ridge model.

```
> lasso.mod <- glmnet(x[train, ], y[train], alpha = 1,
    lambda = grid)
> plot(lasso.mod)
```

We can see from the coefficient plot that depending on the choice of tuning parameter, some of the coefficients will be exactly equal to zero. We now perform cross-validation and compute the associated test error.

```
> set.seed(1)
> cv.out <- cv.glmnet(x[train, ], y[train], alpha = 1)
> plot(cv.out)
> bestlam <- cv.out$lambda.min
> lasso.pred <- predict(lasso.mod, s = bestlam,
    newx = x[test, ])
> mean((lasso.pred - y.test)^2)
[1] 143674
```

This is substantially lower than the test set MSE of the null model and of least squares, and very similar to the test MSE of ridge regression with λ chosen by cross-validation.

However, the lasso has a substantial advantage over ridge regression in that the resulting coefficient estimates are sparse. Here we see that 8 of the 19 coefficient estimates are exactly zero. So the lasso model with λ chosen by cross-validation contains only eleven variables.

```
> out <- glmnet(x, y, alpha = 1, lambda = grid)
> lasso.coef <- predict(out, type = "coefficients",
    s = bestlam)[1:20, ]
> lasso.coef
(Intercept)        AtBat         Hits        HmRun         Runs
       1.27        -0.05         2.18         0.00         0.00
        RBI        Walks        Years       CAtBat        CHits
       0.00         2.29        -0.34         0.00         0.00
     CHmRun        CRuns         CRBI       CWalks     LeagueN
       0.03         0.22         0.42         0.00        20.29
  DivisionW      PutOuts      Assists       Errors   NewLeagueN
    -116.17         0.24         0.00        -0.86         0.00
> lasso.coef[lasso.coef != 0]
(Intercept)        AtBat         Hits        Walks        Years
       1.27        -0.05         2.18         2.29        -0.34
     CHmRun        CRuns         CRBI      LeagueN    DivisionW
       0.03         0.22         0.42        20.29      -116.17
    PutOuts       Errors
       0.24        -0.86
```

6.5.3 PCR and PLS Regression

Principal Components Regression

Principal components regression (PCR) can be performed using the `pcr()` function, which is part of the `pls` library. We now apply PCR to the `Hitters` data, in order to predict `Salary`. Again, we ensure that the missing values have been removed from the data, as described in Section 6.5.1.

`pcr()`

```
> library(pls)
> set.seed(2)
```

```
> pcr.fit <- pcr(Salary ~ ., data = Hitters, scale = TRUE,
    validation = "CV")
```

The syntax for the `pcr()` function is similar to that for `lm()`, with a few additional options. Setting `scale = TRUE` has the effect of *standardizing* each predictor, using (6.6), prior to generating the principal components, so that the scale on which each variable is measured will not have an effect. Setting `validation = "CV"` causes `pcr()` to compute the ten-fold cross-validation error for each possible value of M, the number of principal components used. The resulting fit can be examined using `summary()`.

```
> summary(pcr.fit)
Data:   X dimension: 263 19
        Y dimension: 263 1
Fit method: svdpc
Number of components considered: 19

VALIDATION: RMSEP
Cross-validated using 10 random segments.
       (Intercept)  1 comps  2 comps  3 comps  4 comps
CV             452    351.9    353.2    355.0    352.8
adjCV          452    351.6    352.7    354.4    352.1
...

TRAINING: % variance explained
        1 comps  2 comps  3 comps  4 comps  5 comps
X         38.31    60.16    70.84    79.03    84.29
Salary    40.63    41.58    42.17    43.22    44.90
...
```

The CV score is provided for each possible number of components, ranging from $M = 0$ onwards. (We have printed the CV output only up to $M = 4$.) Note that `pcr()` reports the *root mean squared error*; in order to obtain the usual MSE, we must square this quantity. For instance, a root mean squared error of 352.8 corresponds to an MSE of $352.8^2 = 124{,}468$.

One can also plot the cross-validation scores using the `validationplot()` function. Using `val.type = "MSEP"` will cause the cross-validation MSE to be plotted. `validationplot()`

```
> validationplot(pcr.fit, val.type = "MSEP")
```

We see that the smallest cross-validation error occurs when $M = 18$ components are used. This is barely fewer than $M = 19$, which amounts to simply performing least squares, because when all of the components are used in PCR no dimension reduction occurs. However, from the plot we also see that the cross-validation error is roughly the same when only one component is included in the model. This suggests that a model that uses just a small number of components might suffice.

The `summary()` function also provides the *percentage of variance explained* in the predictors and in the response using different numbers of components. This concept is discussed in greater detail in Chapter 12. Briefly,

we can think of this as the amount of information about the predictors or the response that is captured using M principal components. For example, setting $M = 1$ only captures 38.31 % of all the variance, or information, in the predictors. In contrast, using $M = 5$ increases the value to 84.29 %. If we were to use all $M = p = 19$ components, this would increase to 100 %.

We now perform PCR on the training data and evaluate its test set performance.

```
> set.seed(1)
> pcr.fit <- pcr(Salary ~ ., data = Hitters, subset = train,
    scale = TRUE, validation = "CV")
> validationplot(pcr.fit, val.type = "MSEP")
```

Now we find that the lowest cross-validation error occurs when $M = 5$ components are used. We compute the test MSE as follows.

```
> pcr.pred <- predict(pcr.fit, x[test, ], ncomp = 5)
> mean((pcr.pred - y.test)^2)
[1] 142812
```

This test set MSE is competitive with the results obtained using ridge regression and the lasso. However, as a result of the way PCR is implemented, the final model is more difficult to interpret because it does not perform any kind of variable selection or even directly produce coefficient estimates.

Finally, we fit PCR on the full data set, using $M = 5$, the number of components identified by cross-validation.

```
> pcr.fit <- pcr(y ~ x, scale = TRUE, ncomp = 5)
> summary(pcr.fit)
Data:   X dimension: 263 19
        Y dimension: 263 1
Fit method: svdpc
Number of components considered: 5
TRAINING: % variance explained
   1 comps  2 comps  3 comps  4 comps  5 comps
X    38.31    60.16    70.84    79.03    84.29
y    40.63    41.58    42.17    43.22    44.90
```

Partial Least Squares

We implement partial least squares (PLS) using the `plsr()` function, also in the `pls` library. The syntax is just like that of the `pcr()` function. `plsr()`

```
> set.seed(1)
> pls.fit <- plsr(Salary ~ ., data = Hitters, subset = train, scale
    = TRUE, validation = "CV")
> summary(pls.fit)
Data:   X dimension: 131 19
    Y dimension: 131 1
Fit method: kernelpls
Number of components considered: 19
```

```
VALIDATION: RMSEP
Cross-validated using 10 random segments.
       (Intercept)  1 comps  2 comps  3 comps  4 comps
CV           428.3    325.5    329.9    328.8    339.0
adjCV        428.3    325.0    328.2    327.2    336.6
...

TRAINING: % variance explained
        1 comps  2 comps  3 comps  4 comps  5 comps
X         39.13    48.80    60.09    75.07    78.58
Salary    46.36    50.72    52.23    53.03    54.07
...
> validationplot(pls.fit, val.type = "MSEP")
```

The lowest cross-validation error occurs when only $M = 1$ partial least squares directions are used. We now evaluate the corresponding test set MSE.

```
> pls.pred <- predict(pls.fit, x[test, ], ncomp = 1)
> mean((pls.pred - y.test)^2)
[1] 151995
```

The test MSE is comparable to, but slightly higher than, the test MSE obtained using ridge regression, the lasso, and PCR.

Finally, we perform PLS using the full data set, using $M = 1$, the number of components identified by cross-validation.

```
> pls.fit <- plsr(Salary ~ ., data = Hitters, scale = TRUE,
    ncomp = 1)
> summary(pls.fit)
Data:   X dimension: 263 19
        Y dimension: 263 1
Fit method: kernelpls
Number of components considered: 1
TRAINING: % variance explained
        1 comps
X         38.08
Salary    43.05
```

Notice that the percentage of variance in `Salary` that the one-component PLS fit explains, 43.05 %, is almost as much as that explained using the final five-component model PCR fit, 44.90 %. This is because PCR only attempts to maximize the amount of variance explained in the predictors, while PLS searches for directions that explain variance in both the predictors and the response.

6.6 Exercises

Conceptual

1. We perform best subset, forward stepwise, and backward stepwise selection on a single data set. For each approach, we obtain $p + 1$ models, containing $0, 1, 2, \ldots, p$ predictors. Explain your answers:

   (a) Which of the three models with k predictors has the smallest *training* RSS?

   (b) Which of the three models with k predictors has the smallest *test* RSS?

   (c) True or False:

      i. The predictors in the k-variable model identified by forward stepwise are a subset of the predictors in the $(k+1)$-variable model identified by forward stepwise selection.

      ii. The predictors in the k-variable model identified by backward stepwise are a subset of the predictors in the $(k + 1)$-variable model identified by backward stepwise selection.

      iii. The predictors in the k-variable model identified by backward stepwise are a subset of the predictors in the $(k + 1)$-variable model identified by forward stepwise selection.

      iv. The predictors in the k-variable model identified by forward stepwise are a subset of the predictors in the $(k+1)$-variable model identified by backward stepwise selection.

      v. The predictors in the k-variable model identified by best subset are a subset of the predictors in the $(k + 1)$-variable model identified by best subset selection.

2. For parts (a) through (c), indicate which of i. through iv. is correct. Justify your answer.

   (a) The lasso, relative to least squares, is:

      i. More flexible and hence will give improved prediction accuracy when its increase in bias is less than its decrease in variance.

      ii. More flexible and hence will give improved prediction accuracy when its increase in variance is less than its decrease in bias.

      iii. Less flexible and hence will give improved prediction accuracy when its increase in bias is less than its decrease in variance.

      iv. Less flexible and hence will give improved prediction accuracy when its increase in variance is less than its decrease in bias.

   (b) Repeat (a) for ridge regression relative to least squares.

(c) Repeat (a) for non-linear methods relative to least squares.

3. Suppose we estimate the regression coefficients in a linear regression model by minimizing

$$\sum_{i=1}^{n}\left(y_i-\beta_0-\sum_{j=1}^{p}\beta_j x_{ij}\right)^2 \quad \text{subject to} \quad \sum_{j=1}^{p}|\beta_j|\le s$$

for a particular value of s. For parts (a) through (e), indicate which of i. through v. is correct. Justify your answer.

(a) As we increase s from 0, the training RSS will:
   i. Increase initially, and then eventually start decreasing in an inverted U shape.
   ii. Decrease initially, and then eventually start increasing in a U shape.
   iii. Steadily increase.
   iv. Steadily decrease.
   v. Remain constant.

(b) Repeat (a) for test RSS.

(c) Repeat (a) for variance.

(d) Repeat (a) for (squared) bias.

(e) Repeat (a) for the irreducible error.

4. Suppose we estimate the regression coefficients in a linear regression model by minimizing

$$\sum_{i=1}^{n}\left(y_i-\beta_0-\sum_{j=1}^{p}\beta_j x_{ij}\right)^2+\lambda\sum_{j=1}^{p}\beta_j^2$$

for a particular value of λ. For parts (a) through (e), indicate which of i. through v. is correct. Justify your answer.

(a) As we increase λ from 0, the training RSS will:
   i. Increase initially, and then eventually start decreasing in an inverted U shape.
   ii. Decrease initially, and then eventually start increasing in a U shape.
   iii. Steadily increase.
   iv. Steadily decrease.
   v. Remain constant.

(b) Repeat (a) for test RSS.

(c) Repeat (a) for variance.

(d) Repeat (a) for (squared) bias.

(e) Repeat (a) for the irreducible error.

5. It is well-known that ridge regression tends to give similar coefficient values to correlated variables, whereas the lasso may give quite different coefficient values to correlated variables. We will now explore this property in a very simple setting.

Suppose that $n = 2$, $p = 2$, $x_{11} = x_{12}$, $x_{21} = x_{22}$. Furthermore, suppose that $y_1 + y_2 = 0$ and $x_{11} + x_{21} = 0$ and $x_{12} + x_{22} = 0$, so that the estimate for the intercept in a least squares, ridge regression, or lasso model is zero: $\hat{\beta}_0 = 0$.

(a) Write out the ridge regression optimization problem in this setting.

(b) Argue that in this setting, the ridge coefficient estimates satisfy $\hat{\beta}_1 = \hat{\beta}_2$.

(c) Write out the lasso optimization problem in this setting.

(d) Argue that in this setting, the lasso coefficients $\hat{\beta}_1$ and $\hat{\beta}_2$ are not unique—in other words, there are many possible solutions to the optimization problem in (c). Describe these solutions.

6. We will now explore (6.12) and (6.13) further.

(a) Consider (6.12) with $p = 1$. For some choice of y_1 and $\lambda > 0$, plot (6.12) as a function of β_1. Your plot should confirm that (6.12) is solved by (6.14).

(b) Consider (6.13) with $p = 1$. For some choice of y_1 and $\lambda > 0$, plot (6.13) as a function of β_1. Your plot should confirm that (6.13) is solved by (6.15).

7. We will now derive the Bayesian connection to the lasso and ridge regression discussed in Section 6.2.2.

(a) Suppose that $y_i = \beta_0 + \sum_{j=1}^{p} x_{ij}\beta_j + \epsilon_i$ where $\epsilon_1, \ldots, \epsilon_n$ are independent and identically distributed from a $N(0, \sigma^2)$ distribution. Write out the likelihood for the data.

(b) Assume the following prior for β: $\beta_1, \ldots, \beta_p$ are independent and identically distributed according to a double-exponential distribution with mean 0 and common scale parameter b: i.e. $p(\beta) = \frac{1}{2b}\exp(-|\beta|/b)$. Write out the posterior for β in this setting.

(c) Argue that the lasso estimate is the *mode* for β under this posterior distribution.

(d) Now assume the following prior for β: $\beta_1, \ldots, \beta_p$ are independent and identically distributed according to a normal distribution with mean zero and variance c. Write out the posterior for β in this setting.

(e) Argue that the ridge regression estimate is both the *mode* and the *mean* for β under this posterior distribution.

Applied

8. In this exercise, we will generate simulated data, and will then use this data to perform best subset selection.

(a) Use the `rnorm()` function to generate a predictor X of length $n = 100$, as well as a noise vector ϵ of length $n = 100$.

(b) Generate a response vector Y of length $n = 100$ according to the model

$$Y = \beta_0 + \beta_1 X + \beta_2 X^2 + \beta_3 X^3 + \epsilon,$$

where β_0, β_1, β_2, and β_3 are constants of your choice.

(c) Use the `regsubsets()` function to perform best subset selection in order to choose the best model containing the predictors $X, X^2, \ldots, X^{10}$. What is the best model obtained according to C_p, BIC, and adjusted R^2? Show some plots to provide evidence for your answer, and report the coefficients of the best model obtained. Note you will need to use the `data.frame()` function to create a single data set containing both X and Y.

(d) Repeat (c), using forward stepwise selection and also using backwards stepwise selection. How does your answer compare to the results in (c)?

(e) Now fit a lasso model to the simulated data, again using $X, X^2, \ldots, X^{10}$ as predictors. Use cross-validation to select the optimal value of λ. Create plots of the cross-validation error as a function of λ. Report the resulting coefficient estimates, and discuss the results obtained.

(f) Now generate a response vector Y according to the model

$$Y = \beta_0 + \beta_7 X^7 + \epsilon,$$

and perform best subset selection and the lasso. Discuss the results obtained.

9. In this exercise, we will predict the number of applications received using the other variables in the `College` data set.
   (a) Split the data set into a training set and a test set.
   (b) Fit a linear model using least squares on the training set, and report the test error obtained.
   (c) Fit a ridge regression model on the training set, with λ chosen by cross-validation. Report the test error obtained.
   (d) Fit a lasso model on the training set, with λ chosen by cross-validation. Report the test error obtained, along with the number of non-zero coefficient estimates.
   (e) Fit a PCR model on the training set, with M chosen by cross-validation. Report the test error obtained, along with the value of M selected by cross-validation.
   (f) Fit a PLS model on the training set, with M chosen by cross-validation. Report the test error obtained, along with the value of M selected by cross-validation.
   (g) Comment on the results obtained. How accurately can we predict the number of college applications received? Is there much difference among the test errors resulting from these five approaches?

10. We have seen that as the number of features used in a model increases, the training error will necessarily decrease, but the test error may not. We will now explore this in a simulated data set.
   (a) Generate a data set with $p = 20$ features, $n = 1{,}000$ observations, and an associated quantitative response vector generated according to the model
   $$Y = X\beta + \epsilon,$$
   where β has some elements that are exactly equal to zero.
   (b) Split your data set into a training set containing 100 observations and a test set containing 900 observations.
   (c) Perform best subset selection on the training set, and plot the training set MSE associated with the best model of each size.
   (d) Plot the test set MSE associated with the best model of each size.
   (e) For which model size does the test set MSE take on its minimum value? Comment on your results. If it takes on its minimum value for a model containing only an intercept or a model containing all of the features, then play around with the way that you are generating the data in (a) until you come up with a scenario in which the test set MSE is minimized for an intermediate model size.

(f) How does the model at which the test set MSE is minimized compare to the true model used to generate the data? Comment on the coefficient values.

(g) Create a plot displaying $\sqrt{\sum_{j=1}^{p}(\beta_j - \hat{\beta}_j^r)^2}$ for a range of values of r, where $\hat{\beta}_j^r$ is the jth coefficient estimate for the best model containing r coefficients. Comment on what you observe. How does this compare to the test MSE plot from (d)?

11. We will now try to predict per capita crime rate in the `Boston` data set.

(a) Try out some of the regression methods explored in this chapter, such as best subset selection, the lasso, ridge regression, and PCR. Present and discuss results for the approaches that you consider.

(b) Propose a model (or set of models) that seem to perform well on this data set, and justify your answer. Make sure that you are evaluating model performance using validation set error, cross-validation, or some other reasonable alternative, as opposed to using training error.

(c) Does your chosen model involve all of the features in the data set? Why or why not?