which would imply a totally different relationship among the three conditions. Each of these codings would produce fundamentally different linear models that would ultimately lead to different sets of predictions on test observations.

If the response variable's values did take on a natural ordering, such as *mild*, *moderate*, and *severe*, and we felt the gap between mild and moderate was similar to the gap between moderate and severe, then a 1, 2, 3 coding would be reasonable. Unfortunately, in general there is no natural way to convert a qualitative response variable with more than two levels into a quantitative response that is ready for linear regression.

For a *binary* (two level) qualitative response, the situation is better. For instance, perhaps there are only two possibilities for the patient's medical condition: `stroke` and `drug overdose`. We could then potentially use the *dummy variable* approach from Section 3.3.1 to code the response as follows: binary

$$Y = \begin{cases} 0 & \text{if } \texttt{stroke}; \\ 1 & \text{if } \texttt{drug overdose}. \end{cases}$$

We could then fit a linear regression to this binary response, and predict `drug overdose` if $\hat{Y} > 0.5$ and `stroke` otherwise. In the binary case it is not hard to show that even if we flip the above coding, linear regression will produce the same final predictions.

For a binary response with a 0/1 coding as above, regression by least squares does make sense; it can be shown that the $X\hat{\beta}$ obtained using linear regression is in fact an estimate of $\Pr(\texttt{drug overdose}|X)$ in this special case. However, if we use linear regression, some of our estimates might be outside the $[0, 1]$ interval (see Figure 4.2), making them hard to interpret as probabilities! Nevertheless, the predictions provide an ordering and can be interpreted as crude probability estimates. Curiously, it turns out that the classifications that we get if we use linear regression to predict a binary response will be the same as for the linear discriminant analysis (LDA) procedure we discuss in Section 4.4.

However, the dummy variable approach cannot be easily extended to accommodate qualitative responses with more than two levels. For these reasons, it is preferable to use a classification method that is truly suited for qualitative response values, such as the ones presented next.

4.3 Logistic Regression

Consider again the `Default` data set, where the response `default` falls into one of two categories, `Yes` or `No`. Rather than modeling this response Y directly, logistic regression models the *probability* that Y belongs to a particular category.

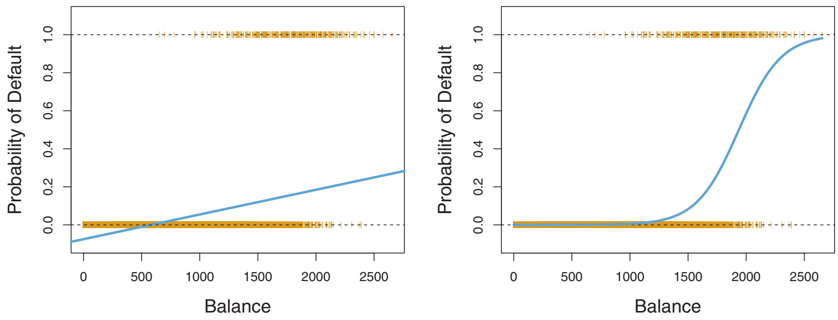

FIGURE 4.2. *Classification using the* `Default` *data.* Left: *Estimated probability of* `default` *using linear regression. Some estimated probabilities are negative! The orange ticks indicate the 0/1 values coded for* `default`*(*`No` *or* `Yes`*).* Right: *Predicted probabilities of* `default` *using logistic regression. All probabilities lie between* 0 *and* 1*.*

For the `Default` data, logistic regression models the probability of default. For example, the probability of default given `balance` can be written as

$$\Pr(\texttt{default} = \texttt{Yes}|\texttt{balance}).$$

The values of $\Pr(\texttt{default} = \texttt{Yes}|\texttt{balance})$, which we abbreviate $p(\texttt{balance})$, will range between 0 and 1. Then for any given value of `balance`, a prediction can be made for `default`. For example, one might predict $\texttt{default} = \texttt{Yes}$ for any individual for whom $p(\texttt{balance}) > 0.5$. Alternatively, if a company wishes to be conservative in predicting individuals who are at risk for default, then they may choose to use a lower threshold, such as $p(\texttt{balance}) > 0.1$.

4.3.1 The Logistic Model

How should we model the relationship between $p(X) = \Pr(Y = 1|X)$ and X? (For convenience we are using the generic 0/1 coding for the response). In Section 4.2 we talked of using a linear regression model to represent these probabilities:

$$p(X) = \beta_0 + \beta_1 X. \tag{4.1}$$

If we use this approach to predict `default=Yes` using `balance`, then we obtain the model shown in the left-hand panel of Figure 4.2. Here we see the problem with this approach: for balances close to zero we predict a negative probability of default; if we were to predict for very large balances, we would get values bigger than 1. These predictions are not sensible, since of course the true probability of default, regardless of credit card balance, must fall between 0 and 1. This problem is not unique to the credit default data. Any time a straight line is fit to a binary response that is coded as

0 or 1, in principle we can always predict $p(X) < 0$ for some values of X and $p(X) > 1$ for others (unless the range of X is limited).

To avoid this problem, we must model $p(X)$ using a function that gives outputs between 0 and 1 for all values of X. Many functions meet this description. In logistic regression, we use the *logistic function*,

logistic function

$$p(X) = \frac{e^{\beta_0+\beta_1 X}}{1 + e^{\beta_0+\beta_1 X}}. \tag{4.2}$$

To fit the model (4.2), we use a method called *maximum likelihood*, which we discuss in the next section. The right-hand panel of Figure 4.2 illustrates the fit of the logistic regression model to the `Default` data. Notice that for low balances we now predict the probability of default as close to, but never below, zero. Likewise, for high balances we predict a default probability close to, but never above, one. The logistic function will always produce an *S-shaped* curve of this form, and so regardless of the value of X, we will obtain a sensible prediction. We also see that the logistic model is better able to capture the range of probabilities than is the linear regression model in the left-hand plot. The average fitted probability in both cases is 0.0333 (averaged over the training data), which is the same as the overall proportion of defaulters in the data set.

maximum likelihood

After a bit of manipulation of (4.2), we find that

$$\frac{p(X)}{1 - p(X)} = e^{\beta_0+\beta_1 X}. \tag{4.3}$$

The quantity $p(X)/[1-p(X)]$ is called the *odds*, and can take on any value between 0 and ∞. Values of the odds close to 0 and ∞ indicate very low and very high probabilities of default, respectively. For example, on average 1 in 5 people with an odds of 1/4 will default, since $p(X) = 0.2$ implies an odds of $\frac{0.2}{1-0.2} = 1/4$. Likewise on average nine out of every ten people with an odds of 9 will default, since $p(X) = 0.9$ implies an odds of $\frac{0.9}{1-0.9} = 9$. Odds are traditionally used instead of probabilities in horse-racing, since they relate more naturally to the correct betting strategy.

odds

By taking the logarithm of both sides of (4.3), we arrive at

$$\log\left(\frac{p(X)}{1 - p(X)}\right) = \beta_0 + \beta_1 X. \tag{4.4}$$

The left-hand side is called the *log-odds* or *logit*. We see that the logistic regression model (4.2) has a logit that is linear in X.

log-odds

logit

Recall from Chapter 3 that in a linear regression model, β_1 gives the average change in Y associated with a one-unit increase in X. In contrast, in a logistic regression model, increasing X by one unit changes the log odds by β_1 (4.4), or equivalently it multiplies the odds by e^{β_1} (4.3). However, because the relationship between $p(X)$ and X in (4.2) is not a straight line,

β_1 does *not* correspond to the change in $p(X)$ associated with a one-unit increase in X. The amount that $p(X)$ changes due to a one-unit change in X will depend on the current value of X. But regardless of the value of X, if β_1 is positive then increasing X will be associated with increasing $p(X)$, and if β_1 is negative then increasing X will be associated with decreasing $p(X)$. The fact that there is not a straight-line relationship between $p(X)$ and X, and the fact that the rate of change in $p(X)$ per unit change in X depends on the current value of X, can also be seen by inspection of the right-hand panel of Figure 4.2.

4.3.2 Estimating the Regression Coefficients

The coefficients β_0 and β_1 in (4.2) are unknown, and must be estimated based on the available training data. In Chapter 3, we used the least squares approach to estimate the unknown linear regression coefficients. Although we could use (non-linear) least squares to fit the model (4.4), the more general method of *maximum likelihood* is preferred, since it has better statistical properties. The basic intuition behind using maximum likelihood to fit a logistic regression model is as follows: we seek estimates for β_0 and β_1 such that the predicted probability $\hat{p}(x_i)$ of default for each individual, using (4.2), corresponds as closely as possible to the individual's observed default status. In other words, we try to find $\hat{\beta}_0$ and $\hat{\beta}_1$ such that plugging these estimates into the model for $p(X)$, given in (4.2), yields a number close to one for all individuals who defaulted, and a number close to zero for all individuals who did not. This intuition can be formalized using a mathematical equation called a *likelihood function*:

likelihood function

$$\ell(\beta_0, \beta_1) = \prod_{i:y_i=1} p(x_i) \prod_{i':y_{i'}=0} (1 - p(x_{i'})). \tag{4.5}$$

The estimates $\hat{\beta}_0$ and $\hat{\beta}_1$ are chosen to *maximize* this likelihood function.

Maximum likelihood is a very general approach that is used to fit many of the non-linear models that we examine throughout this book. In the linear regression setting, the least squares approach is in fact a special case of maximum likelihood. The mathematical details of maximum likelihood are beyond the scope of this book. However, in general, logistic regression and other models can be easily fit using a statistical software package such as `R`, and so we do not need to concern ourselves with the details of the maximum likelihood fitting procedure.

Table 4.1 shows the coefficient estimates and related information that result from fitting a logistic regression model on the `Default` data in order to predict the probability of `default`=`Yes` using `balance`. We see that $\hat{\beta}_1 = 0.0055$; this indicates that an increase in `balance` is associated with an increase in the probability of `default`. To be precise, a one-unit increase in `balance` is associated with an increase in the log odds of `default` by 0.0055 units.

	Coefficient	Std. error	Z-statistic	P-value
`Intercept`	−10.6513	0.3612	−29.5	<0.0001
`balance`	0.0055	0.0002	24.9	<0.0001

TABLE 4.1. *For the* `Default` *data, estimated coefficients of the logistic regression model that predicts the probability of* `default` *using* `balance`*. A one-unit increase in* `balance` *is associated with an increase in the log odds of* `default` *by* 0.0055 *units.*

Many aspects of the logistic regression output shown in Table 4.1 are similar to the linear regression output of Chapter 3. For example, we can measure the accuracy of the coefficient estimates by computing their standard errors. The z-statistic in Table 4.1 plays the same role as the t-statistic in the linear regression output, for example in Table 3.1 on page 68. For instance, the z-statistic associated with β_1 is equal to $\hat{\beta}_1/SE(\hat{\beta}_1)$, and so a large (absolute) value of the z-statistic indicates evidence against the null hypothesis $H_0 : \beta_1 = 0$. This null hypothesis implies that $p(X) = \frac{e^{\beta_0}}{1+e^{\beta_0}}$— in other words, that the probability of `default` does not depend on `balance`. Since the p-value associated with `balance` in Table 4.1 is tiny, we can reject H_0. In other words, we conclude that there is indeed an association between `balance` and probability of `default`. The estimated intercept in Table 4.1 is typically not of interest; its main purpose is to adjust the average fitted probabilities to the proportion of ones in the data.

4.3.3 Making Predictions

Once the coefficients have been estimated, it is a simple matter to compute the probability of `default` for any given credit card balance. For example, using the coefficient estimates given in Table 4.1, we predict that the default probability for an individual with a `balance` of $\$1,000$ is

$$\hat{p}(X) = \frac{e^{\hat{\beta}_0+\hat{\beta}_1 X}}{1+e^{\hat{\beta}_0+\hat{\beta}_1 X}} = \frac{e^{-10.6513+0.0055\times 1,000}}{1+e^{-10.6513+0.0055\times 1,000}} = 0.00576,$$

which is below $1\,\%$. In contrast, the predicted probability of default for an individual with a balance of $\$2,000$ is much higher, and equals 0.586 or $58.6\,\%$.

One can use qualitative predictors with the logistic regression model using the dummy variable approach from Section 3.3.1. As an example, the `Default` data set contains the qualitative variable `student`. To fit the model we simply create a dummy variable that takes on a value of 1 for students and 0 for non-students. The logistic regression model that results from predicting probability of default from student status can be seen in Table 4.2. The coefficient associated with the dummy variable is positive,

	Coefficient	Std. error	Z-statistic	P-value
`Intercept`	−3.5041	0.0707	−49.55	<0.0001
`student[Yes]`	0.4049	0.1150	3.52	0.0004

TABLE 4.2. *For the* `Default` *data, estimated coefficients of the logistic regression model that predicts the probability of* `default` *using student status. Student status is encoded as a dummy variable, with a value of* 1 *for a student and a value of* 0 *for a non-student, and represented by the variable* `student[Yes]` *in the table.*

and the associated p-value is statistically significant. This indicates that students tend to have higher default probabilities than non-students:

$$\widehat{\Pr}(\texttt{default}{=}\texttt{Yes}|\texttt{student}{=}\texttt{Yes}) = \frac{e^{-3.5041+0.4049\times 1}}{1+e^{-3.5041+0.4049\times 1}} = 0.0431,$$
$$\widehat{\Pr}(\texttt{default}{=}\texttt{Yes}|\texttt{student}{=}\texttt{No}) = \frac{e^{-3.5041+0.4049\times 0}}{1+e^{-3.5041+0.4049\times 0}} = 0.0292.$$

4.3.4 Multiple Logistic Regression

We now consider the problem of predicting a binary response using multiple predictors. By analogy with the extension from simple to multiple linear regression in Chapter 3, we can generalize (4.4) as follows:

$$\log\left(\frac{p(X)}{1-p(X)}\right) = \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p, \tag{4.6}$$

where $X = (X_1, \ldots, X_p)$ are p predictors. Equation 4.6 can be rewritten as

$$p(X) = \frac{e^{\beta_0+\beta_1 X_1+\cdots+\beta_p X_p}}{1+e^{\beta_0+\beta_1 X_1+\cdots+\beta_p X_p}}. \tag{4.7}$$

Just as in Section 4.3.2, we use the maximum likelihood method to estimate $\beta_0, \beta_1, \ldots, \beta_p$.

Table 4.3 shows the coefficient estimates for a logistic regression model that uses `balance`, `income` (in thousands of dollars), and `student` status to predict probability of `default`. There is a surprising result here. The p-values associated with `balance` and the dummy variable for `student` status are very small, indicating that each of these variables is associated with the probability of `default`. However, the coefficient for the dummy variable is negative, indicating that students are less likely to default than non-students. In contrast, the coefficient for the dummy variable is positive in Table 4.2. How is it possible for student status to be associated with an *increase* in probability of default in Table 4.2 and a *decrease* in probability of default in Table 4.3? The left-hand panel of Figure 4.3 provides a graphical illustration of this apparent paradox. The orange and blue solid lines show the average default rates for students and non-students, respectively,

	Coefficient	Std. error	Z-statistic	P-value
`Intercept`	−10.8690	0.4923	−22.08	<0.0001
`balance`	0.0057	0.0002	24.74	<0.0001
`income`	0.0030	0.0082	0.37	0.7115
`student[Yes]`	−0.6468	0.2362	−2.74	0.0062

TABLE 4.3. *For the* `Default` *data, estimated coefficients of the logistic regression model that predicts the probability of* `default` *using* `balance`, `income`, *and student status. Student status is encoded as a dummy variable* `student[Yes]`, *with a value of* 1 *for a student and a value of* 0 *for a non-student. In fitting this model,* `income` *was measured in thousands of dollars.*

as a function of credit card balance. The negative coefficient for `student` in the multiple logistic regression indicates that *for a fixed value of* `balance` *and* `income`, a student is less likely to default than a non-student. Indeed, we observe from the left-hand panel of Figure 4.3 that the student default rate is at or below that of the non-student default rate for every value of `balance`. But the horizontal broken lines near the base of the plot, which show the default rates for students and non-students averaged over all values of `balance` and `income`, suggest the opposite effect: the overall student default rate is higher than the non-student default rate. Consequently, there is a positive coefficient for `student` in the single variable logistic regression output shown in Table 4.2.

The right-hand panel of Figure 4.3 provides an explanation for this discrepancy. The variables `student` and `balance` are correlated. Students tend to hold higher levels of debt, which is in turn associated with higher probability of default. In other words, students are more likely to have large credit card balances, which, as we know from the left-hand panel of Figure 4.3, tend to be associated with high default rates. Thus, even though an individual student with a given credit card balance will tend to have a lower probability of default than a non-student with the same credit card balance, the fact that students on the whole tend to have higher credit card balances means that overall, students tend to default at a higher rate than non-students. This is an important distinction for a credit card company that is trying to determine to whom they should offer credit. A student is riskier than a non-student if no information about the student's credit card balance is available. However, that student is less risky than a non-student *with the same credit card balance*!

This simple example illustrates the dangers and subtleties associated with performing regressions involving only a single predictor when other predictors may also be relevant. As in the linear regression setting, the results obtained using one predictor may be quite different from those obtained using multiple predictors, especially when there is correlation among the predictors. In general, the phenomenon seen in Figure 4.3 is known as *confounding*.

confounding

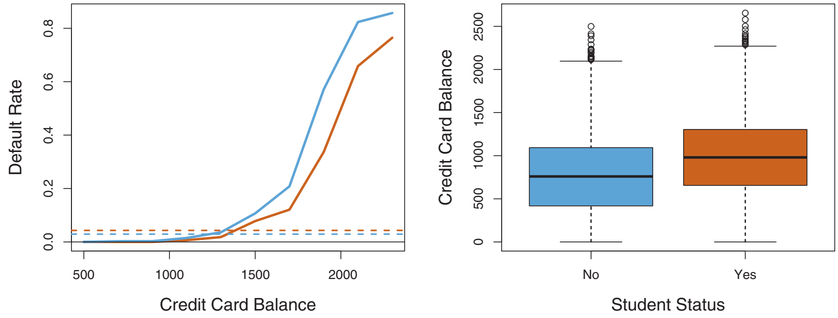

FIGURE 4.3. *Confounding in the* `Default` *data.* Left: *Default rates are shown for students (orange) and non-students (blue). The solid lines display default rate as a function of* `balance`*, while the horizontal broken lines display the overall default rates.* Right: *Boxplots of* `balance` *for students (orange) and non-students (blue) are shown.*

By substituting estimates for the regression coefficients from Table 4.3 into (4.7), we can make predictions. For example, a student with a credit card balance of \$1,500 and an income of \$40,000 has an estimated probability of default of

$$\hat{p}(X) = \frac{e^{-10.869+0.00574\times 1{,}500+0.003\times 40-0.6468\times 1}}{1+e^{-10.869+0.00574\times 1{,}500+0.003\times 40-0.6468\times 1}} = 0.058. \tag{4.8}$$

A non-student with the same balance and income has an estimated probability of default of

$$\hat{p}(X) = \frac{e^{-10.869+0.00574\times 1{,}500+0.003\times 40-0.6468\times 0}}{1+e^{-10.869+0.00574\times 1{,}500+0.003\times 40-0.6468\times 0}} = 0.105. \tag{4.9}$$

(Here we multiply the `income` coefficient estimate from Table 4.3 by 40, rather than by 40,000, because in that table the model was fit with `income` measured in units of \$1,000.)

4.3.5 Logistic Regression for >2 Response Classes

We sometimes wish to classify a response variable that has more than two classes. For example, in Section 4.2 we had three categories of medical condition in the emergency room: `stroke`, `drug overdose`, `epileptic seizure`. In this setting, we wish to model both $\Pr(Y = \texttt{stroke}|X)$ and $\Pr(Y = \texttt{drug overdose}|X)$, with the remaining $\Pr(Y = \texttt{epileptic seizure}|X) = 1 - \Pr(Y = \texttt{stroke}|X) - \Pr(Y = \texttt{drug overdose}|X)$. The two-class logistic regression models discussed in the previous sections have multiple-class extensions, but in practice they tend not to be used all that often. One of the reasons is that the method we discuss in the next section, *discriminant*