4
Classification

The linear regression model discussed in Chapter 3 assumes that the response variable Y is quantitative. But in many situations, the response variable is instead *qualitative*. For example, eye color is qualitative. Often qualitative variables are referred to as *categorical*; we will use these terms interchangeably. In this chapter, we study approaches for predicting qualitative responses, a process that is known as *classification*. Predicting a qualitative response for an observation can be referred to as *classifying* that observation, since it involves assigning the observation to a category, or class. On the other hand, often the methods used for classification first predict the probability that the observation belongs to each of the categories of a qualitative variable, as the basis for making the classification. In this sense they also behave like regression methods.

qualitative

classification

There are many possible classification techniques, or *classifiers*, that one might use to predict a qualitative response. We touched on some of these in Sections 2.1.5 and 2.2.3. In this chapter we discuss some widely-used classifiers: *logistic regression*, *linear discriminant analysis*, *quadratic discriminant analysis*, *naive Bayes*, and K*-nearest neighbors*. The discussion of logistic regression is used as a jumping-off point for a discussion of *generalized linear models*, and in particular, *Poisson regression*. We discuss more computer-intensive classification methods in later chapters: these include generalized additive models (Chapter 7); trees, random forests, and boosting (Chapter 8); and support vector machines (Chapter 9).

classifier

logistic regression

linear discriminant analysis

quadratic discriminant analysis

naive Bayes

K-nearest neighbors

generalized linear models

Poisson regression

4.1 An Overview of Classification

Classification problems occur often, perhaps even more so than regression problems. Some examples include:

G. James et al., *An Introduction to Statistical Learning*, Springer Texts in Statistics,
https://doi.org/10.1007/978-3-031-38747-0_4

1. A person arrives at the emergency room with a set of symptoms that could possibly be attributed to one of three medical conditions. Which of the three conditions does the individual have?

2. An online banking service must be able to determine whether or not a transaction being performed on the site is fraudulent, on the basis of the user's IP address, past transaction history, and so forth.

3. On the basis of DNA sequence data for a number of patients with and without a given disease, a biologist would like to figure out which DNA mutations are deleterious (disease-causing) and which are not.

Just as in the regression setting, in the classification setting we have a set of training observations $(x_1, y_1), \ldots, (x_n, y_n)$ that we can use to build a classifier. We want our classifier to perform well not only on the training data, but also on test observations that were not used to train the classifier.

In this chapter, we will illustrate the concept of classification using the simulated `Default` data set. We are interested in predicting whether an individual will default on his or her credit card payment, on the basis of annual income and monthly credit card balance. The data set is displayed in Figure 4.1. In the left-hand panel of Figure 4.1, we have plotted annual `income` and monthly credit card `balance` for a subset of $10,000$ individuals. The individuals who defaulted in a given month are shown in orange, and those who did not in blue. (The overall default rate is about $3\,\%$, so we have plotted only a fraction of the individuals who did not default.) It appears that individuals who defaulted tended to have higher credit card balances than those who did not. In the center and right-hand panels of Figure 4.1, two pairs of boxplots are shown. The first shows the distribution of `balance` split by the binary `default` variable; the second is a similar plot for `income`. In this chapter, we learn how to build a model to predict `default` (Y) for any given value of `balance` (X_1) and `income` (X_2). Since Y is not quantitative, the simple linear regression model of Chapter 3 is not a good choice: we will elaborate on this further in Section 4.2.

It is worth noting that Figure 4.1 displays a very pronounced relationship between the predictor `balance` and the response `default`. In most real applications, the relationship between the predictor and the response will not be nearly so strong. However, for the sake of illustrating the classification procedures discussed in this chapter, we use an example in which the relationship between the predictor and the response is somewhat exaggerated.

4.2 Why Not Linear Regression?

We have stated that linear regression is not appropriate in the case of a qualitative response. Why not?

Suppose that we are trying to predict the medical condition of a patient in the emergency room on the basis of her symptoms. In this simplified example, there are three possible diagnoses: `stroke`, `drug overdose`, and

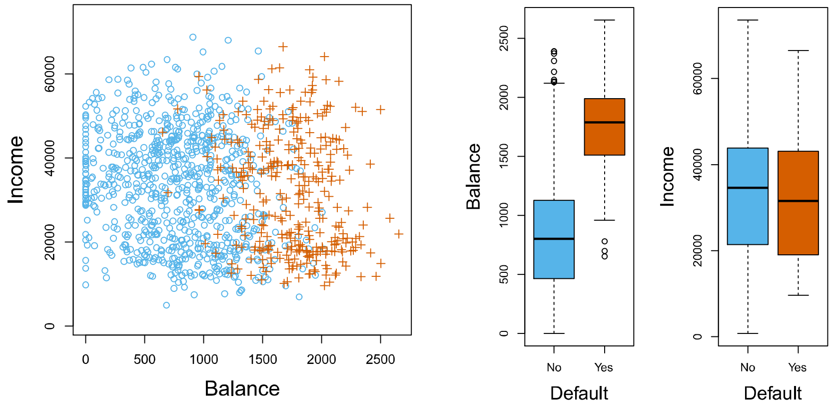

FIGURE 4.1. *The* `Default` *data set.* Left: *The annual incomes and monthly credit card balances of a number of individuals. The individuals who defaulted on their credit card payments are shown in orange, and those who did not are shown in blue.* Center: *Boxplots of* `balance` *as a function of* `default` *status.* Right: *Boxplots of* `income` *as a function of* `default` *status.*

`epileptic seizure`. We could consider encoding these values as a quantitative response variable, Y, as follows:

$$Y = \begin{cases} 1 & \text{if } \texttt{stroke}; \\ 2 & \text{if } \texttt{drug overdose}; \\ 3 & \text{if } \texttt{epileptic seizure}. \end{cases}$$

Using this coding, least squares could be used to fit a linear regression model to predict Y on the basis of a set of predictors $X_1, \ldots, X_p$. Unfortunately, this coding implies an ordering on the outcomes, putting `drug overdose` in between `stroke` and `epileptic seizure`, and insisting that the difference between `stroke` and `drug overdose` is the same as the difference between `drug overdose` and `epileptic seizure`. In practice there is no particular reason that this needs to be the case. For instance, one could choose an equally reasonable coding,

$$Y = \begin{cases} 1 & \text{if } \texttt{epileptic seizure}; \\ 2 & \text{if } \texttt{stroke}; \\ 3 & \text{if } \texttt{drug overdose}, \end{cases}$$

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 is not completely unreasonable: 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.

To summarize, there are at least two reasons not to perform classification using a regression method: (a) a regression method cannot accommodate a qualitative response with more than two classes; (b) a regression method will not provide meaningful estimates of $\Pr(Y|X)$, even with just two classes. Thus, it is preferable to use a classification method that is truly suited for qualitative response values. In the next section, we present logistic regression, which is well-suited for the case of a binary qualitative response; in later sections we will cover classification methods that are appropriate when the qualitative response has two or more classes.

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.

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 default $=$ Yes

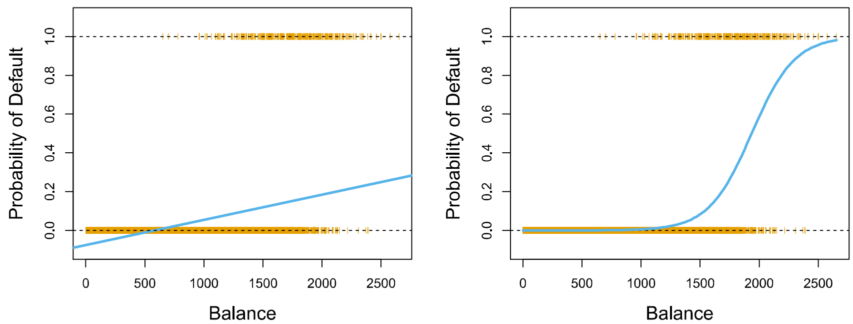

FIGURE 4.2. *Classification using the* `Default` *data.* Left: *Estimated probability of* `default` *using linear regression. Some estimated probabilities are negative! The orange ticks indicate the 0/1 values coded for* `default` *(*`No` *or* `Yes`*).* Right: *Predicted probabilities of* `default` *using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

for any individual for whom $p($`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 $p($`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 considered 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

maximum likelihood

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.

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. By contrast, in a logistic regression model, increasing X by one unit changes the log odds by β_1 (4.4). 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 depends 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 statistical software 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.

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 77. For instance, the z-statistic associated with β_1 is equal to $\hat{\beta}_1/\mathrm{SE}(\hat{\beta}_1)$, 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 (in this case, the overall default rate).

4.3.3 Making Predictions

Once the coefficients have been estimated, we can 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

	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.*

	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.*

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 a model that uses student status as a predictor variable, 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, 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

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

	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.*

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, 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

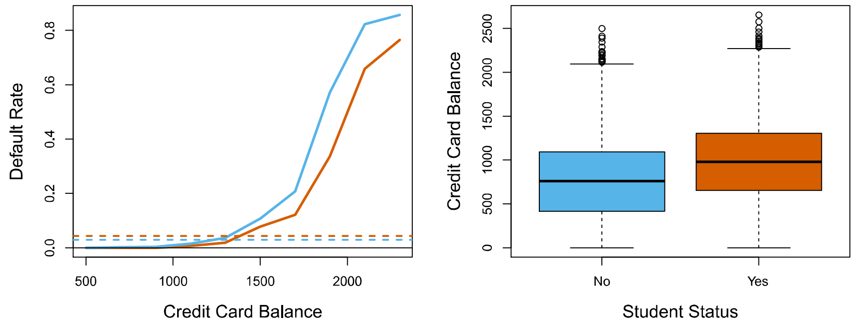

FIGURE 4.3. *Confounding in the* `Default` *data.* Left: *Default rates are shown for students (orange) and non-students (blue). The solid lines display default rate as a function of* `balance`*, while the horizontal broken lines display the overall default rates.* Right: *Boxplots of* `balance` *for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

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

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 Multinomial Logistic Regression

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`. However, the logistic regression approach that we have seen in this section only allows for $K = 2$ classes for the response variable.

It turns out that it is possible to extend the two-class logistic regression approach to the setting of $K > 2$ classes. This extension is sometimes known as *multinomial logistic regression*. To do this, we first select a single class to serve as the *baseline*; without loss of generality, we select the Kth class for this role. Then we replace the model (4.7) with the model

multinomial logistic regression

$$\Pr(Y = k|X = x) = \frac{e^{\beta_{k0}+\beta_{k1}x_1+\cdots+\beta_{kp}x_p}}{1 + \sum_{l=1}^{K-1} e^{\beta_{l0}+\beta_{l1}x_1+\cdots+\beta_{lp}x_p}} \tag{4.10}$$

for $k = 1, \ldots, K-1$, and

$$\Pr(Y = K|X = x) = \frac{1}{1 + \sum_{l=1}^{K-1} e^{\beta_{l0}+\beta_{l1}x_1+\cdots+\beta_{lp}x_p}}. \tag{4.11}$$

It is not hard to show that for $k = 1, \ldots, K-1$,

$$\log\left(\frac{\Pr(Y = k|X = x)}{\Pr(Y = K|X = x)}\right) = \beta_{k0} + \beta_{k1}x_1 + \cdots + \beta_{kp}x_p. \tag{4.12}$$

Notice that (4.12) is quite similar to (4.6). Equation 4.12 indicates that once again, the log odds between any pair of classes is linear in the features.

It turns out that in (4.10)–(4.12), the decision to treat the Kth class as the baseline is unimportant. For example, when classifying emergency room visits into `stroke`, `drug overdose`, and `epileptic seizure`, suppose that we fit two multinomial logistic regression models: one treating `stroke` as the baseline, another treating `drug overdose` as the baseline. The coefficient estimates will differ between the two fitted models due to the differing choice of baseline, but the fitted values (predictions), the log odds between any pair of classes, and the other key model outputs will remain the same.

Nonetheless, interpretation of the coefficients in a multinomial logistic regression model must be done with care, since it is tied to the choice of baseline. For example, if we set `epileptic seizure` to be the baseline, then we can interpret $\beta_{\texttt{stroke}0}$ as the log odds of `stroke` versus `epileptic seizure`, given that $x_1 = \cdots = x_p = 0$. Furthermore, a one-unit increase in X_j is associated with a $\beta_{\texttt{stroke}j}$ increase in the log odds of `stroke` over `epileptic seizure`. Stated another way, if X_j increases by one unit, then

$$\frac{\Pr(Y = \texttt{stroke}|X = x)}{\Pr(Y = \texttt{epileptic seizure}|X = x)}$$

increases by $e^{\beta_{\texttt{stroke}j}}$.

We now briefly present an alternative coding for multinomial logistic regression, known as the *softmax* coding. The softmax coding is equivalent to the coding just described in the sense that the fitted values, log odds between any pair of classes, and other key model outputs will remain the same, regardless of coding. But the softmax coding is used extensively in some areas of the machine learning literature (and will appear again in Chapter 10), so it is worth being aware of it. In the softmax coding, rather than selecting a baseline class, we treat all K classes symmetrically, and assume that for $k = 1, \ldots, K$,

softmax

$$\Pr(Y = k|X = x) = \frac{e^{\beta_{k0}+\beta_{k1}x_1+\cdots+\beta_{kp}x_p}}{\sum_{l=1}^{K} e^{\beta_{l0}+\beta_{l1}x_1+\cdots+\beta_{lp}x_p}}. \tag{4.13}$$

Thus, rather than estimating coefficients for $K-1$ classes, we actually estimate coefficients for all K classes. It is not hard to see that as a result of (4.13), the log odds ratio between the kth and k'th classes equals

$$\log\left(\frac{\Pr(Y=k|X=x)}{\Pr(Y=k'|X=x)}\right) = (\beta_{k0}-\beta_{k'0}) + (\beta_{k1}-\beta_{k'1})x_1 + \cdots + (\beta_{kp}-\beta_{k'p})x_p. \tag{4.14}$$

4.4 Generative Models for Classification

Logistic regression involves directly modeling $\Pr(Y=k|X=x)$ using the logistic function, given by (4.7) for the case of two response classes. In statistical jargon, we model the conditional distribution of the response Y, given the predictor(s) X. We now consider an alternative and less direct approach to estimating these probabilities. In this new approach, we model the distribution of the predictors X separately in each of the response classes (i.e. for each value of Y). We then use Bayes' theorem to flip these around into estimates for $\Pr(Y=k|X=x)$. When the distribution of X within each class is assumed to be normal, it turns out that the model is very similar in form to logistic regression.

Why do we need another method, when we have logistic regression? There are several reasons:

- When there is substantial separation between the two classes, the parameter estimates for the logistic regression model are surprisingly unstable. The methods that we consider in this section do not suffer from this problem.
- If the distribution of the predictors X is approximately normal in each of the classes and the sample size is small, then the approaches in this section may be more accurate than logistic regression.
- The methods in this section can be naturally extended to the case of more than two response classes. (In the case of more than two response classes, we can also use multinomial logistic regression from Section 4.3.5.)

Suppose that we wish to classify an observation into one of K classes, where $K \geq 2$. In other words, the qualitative response variable Y can take on K possible distinct and unordered values. Let π_k represent the overall or *prior* probability that a randomly chosen observation comes from the kth class. Let $f_k(X) \equiv \Pr(X|Y=k)$[1] denote the *density function* of X for an observation that comes from the kth class. In other words, $f_k(x)$ is relatively large if there is a high probability that an observation in the kth class has $X \approx x$, and $f_k(x)$ is small if it is very unlikely that an observation in the kth class has $X \approx x$. Then *Bayes' theorem* states that

prior

density function

Bayes' theorem

[1]Technically, this definition is only correct if X is a qualitative random variable. If X is quantitative, then $f_k(x)dx$ corresponds to the probability of X falling in a small region dx around x.

$$\Pr(Y = k|X = x) = \frac{\pi_k f_k(x)}{\sum_{l=1}^{K} \pi_l f_l(x)}. \tag{4.15}$$

In accordance with our earlier notation, we will use the abbreviation $p_k(x) = \Pr(Y = k|X = x)$; this is the *posterior* probability that an observation $X = x$ belongs to the kth class. That is, it is the probability that the observation belongs to the kth class, *given* the predictor value for that observation.

posterior

Equation 4.15 suggests that instead of directly computing the posterior probability $p_k(x)$ as in Section 4.3.1, we can simply plug in estimates of π_k and $f_k(x)$ into (4.15). In general, estimating π_k is easy if we have a random sample from the population: we simply compute the fraction of the training observations that belong to the kth class. However, estimating the density function $f_k(x)$ is much more challenging. As we will see, to estimate $f_k(x)$, we will typically have to make some simplifying assumptions.

We know from Chapter 2 that the Bayes classifier, which classifies an observation x to the class for which $p_k(x)$ is largest, has the lowest possible error rate out of all classifiers. (Of course, this is only true if all of the terms in (4.15) are correctly specified.) Therefore, if we can find a way to estimate $f_k(x)$, then we can plug it into (4.15) in order to approximate the Bayes classifier.

In the following sections, we discuss three classifiers that use different estimates of $f_k(x)$ in (4.15) to approximate the Bayes classifier: *linear discriminant analysis, quadratic discriminant analysis,* and *naive Bayes*.

4.4.1 Linear Discriminant Analysis for $p = 1$

For now, assume that $p = 1$—that is, we have only one predictor. We would like to obtain an estimate for $f_k(x)$ that we can plug into (4.15) in order to estimate $p_k(x)$. We will then classify an observation to the class for which $p_k(x)$ is greatest. To estimate $f_k(x)$, we will first make some assumptions about its form.

In particular, we assume that $f_k(x)$ is *normal* or *Gaussian*. In the one-dimensional setting, the normal density takes the form

normal
Gaussian

$$f_k(x) = \frac{1}{\sqrt{2\pi}\sigma_k} \exp\left(-\frac{1}{2\sigma_k^2}(x - \mu_k)^2\right), \tag{4.16}$$

where μ_k and σ_k^2 are the mean and variance parameters for the kth class. For now, let us further assume that $\sigma_1^2 = \cdots = \sigma_K^2$: that is, there is a shared variance term across all K classes, which for simplicity we can denote by σ^2. Plugging (4.16) into (4.15), we find that

$$p_k(x) = \frac{\pi_k \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{1}{2\sigma^2}(x - \mu_k)^2\right)}{\sum_{l=1}^{K} \pi_l \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{1}{2\sigma^2}(x - \mu_l)^2\right)}. \tag{4.17}$$

(Note that in (4.17), π_k denotes the prior probability that an observation belongs to the kth class, not to be confused with $\pi \approx 3.14159$, the mathematical constant.) The Bayes classifier[2] involves assigning an observation

[2]Recall that the *Bayes classifier* assigns an observation to the class for which $p_k(x)$ is largest. This is different from *Bayes' theorem* in (4.15), which allows us to manipulate conditional distributions.