

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

$$Y \approx \beta_0 + \beta_1 X. \quad (3.1)$$

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

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

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

$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x, \quad (3.2)$$

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

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

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 $i = 1, \dots, n$. 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

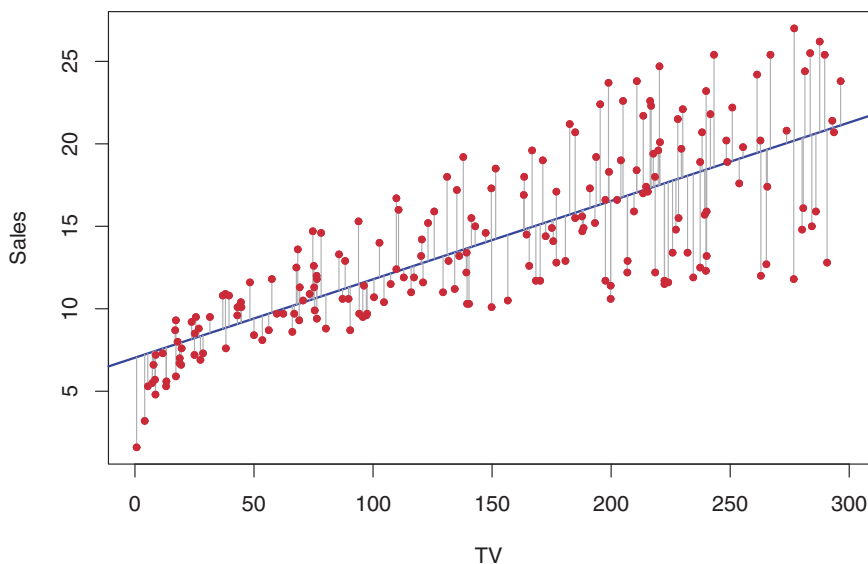


FIGURE 3.1. For the **Advertising** data, the least squares fit for the regression of **sales** onto **TV** is shown. The fit is found by minimizing the sum of squared errors. Each grey line segment represents an error, and the fit makes a compromise by averaging their squares. In this case a linear fit captures the essence of the relationship, although it is somewhat deficient 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 i th value of X . Then $e_i = y_i - \hat{y}_i$ represents the i th *residual*—this is the difference between the i th observed response value and the i th response value that is predicted by our linear model. We define the *residual sum of squares* (RSS) as

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

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

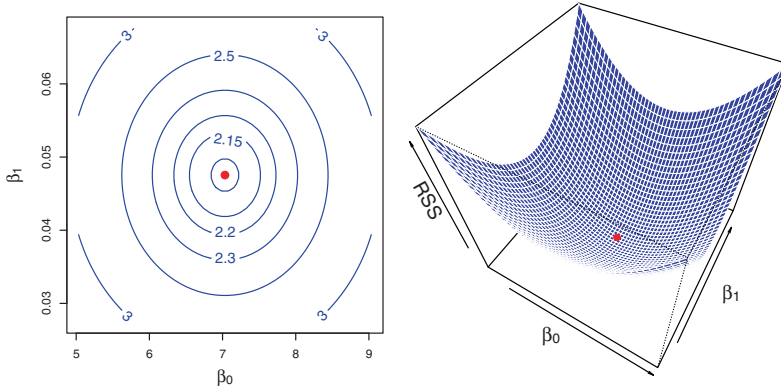


FIGURE 3.2. Contour and three-dimensional plots of the RSS on the **Advertising** data, using **sales** as the response and **TV** as the predictor. The red dots correspond to the least squares estimates $\hat{\beta}_0$ and $\hat{\beta}_1$, given by (3.4).

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

$$Y = \beta_0 + \beta_1 X + \epsilon. \quad (3.5)$$

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 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

population
regression
line

least squares
line

¹The 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.

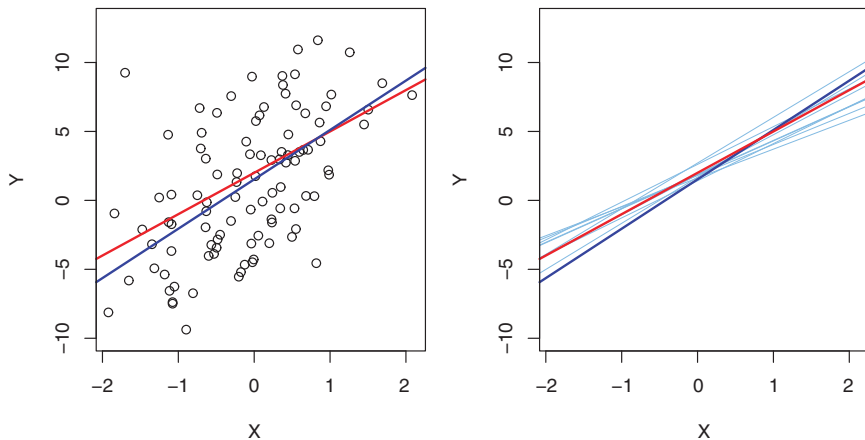


FIGURE 3.3. A simulated data set. Left: The red line represents the true relationship, $f(X) = 2 + 3X$, which is known as the population regression line. The blue line is the least squares line; it is the least squares estimate for $f(X)$ based on the observed data, shown in black. Right: The population 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.

two lines in a simple simulated example. We created 100 random X s, and generated 100 corresponding Y s from the model

$$Y = 2 + 3X + \epsilon, \quad (3.6)$$

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.

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 , which we can write as y_1, \dots, y_n , and 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, \dots, 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.

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 $SE(\hat{\mu})$. We have the well-known formula

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

bias
unbiased

standard
error

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:

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

where $\sigma^2 = \text{Var}(\epsilon)$. For these formulas to be strictly valid, we need to assume that the errors ϵ_i for each observation are uncorrelated with common variance σ^2 . 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 $\text{SE}(\hat{\beta}_1)$ 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 $\text{SE}(\hat{\beta}_0)$ would be the same as $\text{SE}(\hat{\mu})$ 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. The estimate of σ is known as the *residual standard error*, and is given by the formula $\text{RSE} = \sqrt{\text{RSS}/(n-2)}$. Strictly speaking, when σ^2 is estimated from the data we should write $\widehat{\text{SE}}(\hat{\beta}_1)$ 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. For linear regression, the 95% confidence interval for β_1 approximately takes the form

confidence
interval

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

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

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

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

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

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

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.

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 7,940 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

$$H_0 : \text{There is no relationship between } X \text{ and } Y \quad (3.12) \quad \text{null hypothesis}$$

versus the *alternative hypothesis*

$$H_a : \text{There is some relationship between } X \text{ and } Y. \quad (3.13) \quad \text{alternative hypothesis}$$

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*, t-statistic given by

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

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 normal distribution. Consequently, it is a simple matter to compute the probability of observing any value equal to $|t|$ or larger, 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, 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%. When $n = 30$, these correspond to t-statistics (3.14) of around 2 and 2.75, respectively.

	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).

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

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

⁴In 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.