## Chapter 17

## Linear Regression

Linear regression is a statistical method for examining the relationship between two continuous variables, typically called $Y$ and $X$. It assumes a linear relationship between the two variables, with a slope and intercept. One common purpose of linear regression is to establish whether changes in $X$ cause changes in $Y$, by testing whether the slope of this line is significantly different from zero. Another purpose is prediction. Given a value of $X$, linear regression can be used to predict the value of $Y$ and generate a confidence interval for this prediction. The variable $X$ is sometimes under the control of the investigator, similar to a fixed effect in ANOVA, but can also be a random variable.

A basic assumption of linear regression is that $X$ could be causing changes in $Y$, but not the reverse. For this reason, $Y$ is often called the dependent variable while $X$ is the independent variable in the analysis. The term regressor is also used for the independent variable in this context. For example, we might be interested in the effect of temperature on the growth rate of fish. Temperature might cause an increased growth rate, but clearly growth rate cannot influence temperature. This causal relationship is a distinguishing feature of regression as opposed to correlation analysis. Correlation is used to examine the association between two continuous variables and no causal direction is assumed (see Chapter 18). For example, we might be interested in the relationship between fish length and weight but there is no obvious causal relationship between the two variables.

Although linear regression assumes a different statistical model than ANOVA, there are a number of similarities in the estimation process and statistical tests for the two types. For example, both ANOVA and linear regression
models use likelihood methods for parameter estimation and test construction, and employ $F$ statistics to test various hypotheses. Both are examples of general linear models, in which the model parameters and error terms enter the model in an additive (linear) fashion.

What do the data look like for linear regression? As an example, we will use data from study on the southern pine beetle, Dendroctonus frontalis (Reeve et al. 1998). The study used cages to experimentally manipulate the density of $D$. frontalis attacking pine trees. The independent or $X$ variable in the study was the number of beetles added to the cages, while the dependent or $Y$ variable was the number of attacks the beetles made through the bark into the tree (Table 17.1). The notation $Y_{i}$ and $X_{i}$ refers to the values for the $i t h$ pair of numbers. For example, $Y_{2}=2.660$ and $X_{2}=1.000$. We will later see there is a positive relationship between the two variables, with attack density increasing as more beetles are added to the cages. Besides establishing the relationship between the two variables, there was also some interest in predicting the attack density as a function of the number of beetles added to the cage, for use in future studies. We will use the linear regression model to predict attack density for $X=1.75$, a value not occurring in the data set.

Table 17.1: Example 1 - Observations from an experiment in which different numbers of the bark beetle $D$. frontalis were introduced into cages and the resulting attack density recorded (Reeve et al. 1998). Here $Y$ is the attack density (attacks per $100 \mathrm{~cm}^{2}$ of bark) while $X$ is the number of beetles added $\left(\times 10^{3}\right)$. Also shown are some preliminary calculations for the regression analysis.

| $i$ | $Y_{i}$ | $X_{i}$ | $\left(X_{i}-\bar{X}\right)^{2}$ | $\left(Y_{i}-\bar{Y}\right)\left(X_{i}-\bar{X}\right)$ | $\hat{Y}_{i}=\hat{\alpha}+\hat{\beta} X_{i}$ | $Y_{i}-\hat{Y}_{i}$ | $\left(Y_{i}-\hat{Y}_{i}\right)^{2}$ | $\left(\hat{Y}_{i}-\bar{Y}\right)^{2}$ | $\left(Y_{i}-\bar{Y}\right)^{2}$ |
| ---: | :---: | ---: | ---: | ---: | ---: | ---: | ---: | ---: | ---: | ---: |
| 1 | 1.250 | 0.100 | 0.740 | 2.779 | 2.206 | -0.956 | 0.914 | 5.176 | 10.440 |
| 2 | 2.660 | 1.000 | 0.002 | -0.073 | 4.586 | -1.926 | 3.711 | 0.011 | 3.316 |
| 3 | 7.330 | 2.000 | 1.081 | 2.962 | 7.231 | 0.099 | 0.010 | 7.563 | 8.116 |
| 4 | 1.600 | 1.250 | 0.084 | -0.835 | 5.248 | -3.648 | 13.305 | 0.588 | 8.301 |
| 5 | 2.620 | 0.500 | 0.212 | 0.856 | 3.264 | -0.644 | 0.415 | 1.481 | 3.464 |
| 6 | 1.000 | 0.200 | 0.578 | 2.646 | 2.471 | -1.471 | 2.162 | 4.042 | 12.118 |
| 7 | 4.340 | 1.500 | 0.291 | -0.076 | 5.909 | -1.569 | 2.461 | 2.038 | 0.020 |
| 8 | 5.230 | 0.750 | 0.044 | -0.157 | 3.925 | 1.305 | 1.702 | 0.309 | 0.561 |
| 9 | 2.500 | 0.250 | 0.504 | 1.407 | 2.603 | -0.103 | 0.011 | 3.528 | 3.925 |
| 10 | 3.250 | 0.500 | 0.212 | 0.567 | 3.264 | -0.014 | 0.000 | 1.481 | 1.516 |
| 11 | 6.000 | 2.000 | 1.081 | 1.579 | 7.231 | -1.231 | 1.516 | 7.563 | 2.307 |
| 12 | 4.750 | 1.500 | 0.291 | 0.145 | 5.909 | -1.159 | 1.343 | 2.038 | 0.072 |
| 13 | 2.500 | 0.250 | 0.504 | 1.407 | 2.603 | -0.103 | 0.011 | 3.528 | 3.925 |
| 14 | 8.750 | 2.000 | 1.081 | 4.439 | 7.231 | 1.519 | 2.307 | 7.563 | 18.223 |
| 15 | 6.000 | 1.000 | 0.002 | 0.060 | 4.586 | 1.414 | 1.998 | 0.011 | 2.307 |
| 16 | 5.000 | 0.500 | 0.212 | -0.239 | 3.264 | 1.736 | 3.014 | 1.481 | 0.269 |
| 17 | 7.150 | 1.000 | 0.002 | 0.106 | 4.586 | 2.564 | 6.572 | 0.011 | 7.123 |
| 18 | 6.750 | 1.500 | 0.291 | 1.225 | 5.909 | 0.841 | 0.708 | 2.038 | 5.158 |
| 19 | 7.500 | 1.500 | 0.291 | 1.630 | 5.909 | 1.591 | 2.532 | 2.038 | 9.114 |
| 20 | 2.500 | 0.500 | 0.212 | 0.912 | 3.264 | -0.764 | 0.584 | 1.481 | 3.920 .5 |
| 21 | 5.000 | 2.000 | 1.081 | 0.540 | 7.231 | -2.231 | 4.979 | 7.563 | 0.269 |
| 22 | 2.250 | 0.250 | 0.504 | 1.585 | 2.603 | -0.353 | 0.124 | 3.528 | 4.978 |


|  |  |  |  |  |  |  |  |  |  |
| ---: | ---: | ---: | ---: | ---: | ---: | ---: | ---: | ---: | ---: | ---: |
| $i$ | $Y_{i}$ | $X_{i}$ | $\left(X_{i}-\bar{X}\right)^{2}$ | $\left(Y_{i}-\bar{Y}\right)\left(X_{i}-\bar{X}\right)$ | $\hat{Y}_{i}=\hat{\alpha}+\hat{\beta} X_{i}$ | $Y_{i}-\hat{Y}_{i}$ | $\left(Y_{i}-\hat{Y}_{i}\right)^{2}$ | $\left(\hat{Y}_{i}-\bar{Y}\right)^{2}$ | $\left(Y_{i}-\bar{Y}\right)^{2}$ |
| 23 | 1.250 | 0.125 | 0.698 | 2.699 | 2.272 | -1.022 | 1.045 | 4.879 | 10.440 |
| 24 | 4.750 | 1.000 | 0.002 | 0.011 | 4.586 | 0.164 | 0.027 | 0.011 | 0.072 |
| 25 | 4.500 | 0.250 | 0.504 | -0.013 | 2.603 | 1.897 | 3.599 | 3.528 | 0.000 |
| 26 | 9.560 | 2.000 | 1.081 | 5.281 | 7.231 | 2.329 | 5.423 | 7.563 | 25.795 |
| 27 | 5.000 | 0.500 | 0.212 | -0.239 | 3.264 | 1.736 | 3.014 | 1.481 | 0.269 |
| $\sum$ |  |  | 11.798 | 31.203 |  |  | 63.486 | 82.528 | 146.014 |

CHAPTER 17. LINEAR REGRESSION

### 17.1 Linear regression model

Suppose that we want to model the observations in studies like Example 1, where $Y$ is observed for a number of $X$ values. Let $Y_{i}$ and $X_{i}$ stand for the $i$ th pair of values. The linear regression model takes the form

$$
\begin{equation*}
Y_{i}=\alpha+\beta X_{i}+\epsilon_{i}, \tag{17.1}
\end{equation*}
$$

where $\alpha$ is the intercept and $\beta$ the slope of a line, while $\epsilon_{i} \sim N\left(0, \sigma^{2}\right)$ (Searle 1971). Thus, the linear regression model represents the relationship between $Y_{i}$ and $X_{i}$ as a line on which random deviations due to natural variability $\left(\epsilon_{i}\right)$ are imposed. The slope $\beta$ is also called the regression coefficient.

For the $i$ th pair of values, we have $E\left[Y_{i}\right]=\alpha+\beta X_{i}$ and $\operatorname{Var}\left[Y_{i}\right]=\sigma^{2}$ using the rules for expected values and variances. Thus, $Y_{i} \sim N\left(\alpha+\beta X_{i}, \sigma^{2}\right)$ for any $X_{i}$ value. The behavior of the linear regression model can be illustrated by plotting this distribution across a range of $X_{i}$ values. When $\beta$ is positive, the mean of $Y_{i}$ will increase as $X_{i}$ increases (Fig. 17.1), while if $\beta$ is negative the mean would decrease (not shown). The variance remains the same for all $X_{i}$. Note that the linear regression model has assumptions similar to the ANOVA models - the observations are assumed be normal and have the same variance.

The first objective in linear regression is to estimate the model parameters, especially the slope $\beta$, and then test whether it is different from zero. In particular, we will be interested in testing $H_{0}: \beta=0$. If a test of this hypothesis is significant this suggests a causal relationship (positive or negative) between $Y$ and $X$. The alternative hypothesis can be written as $H_{1}: \beta \neq 0$. It is also possible to test whether the intercept differs from zero although this is less common. We will discuss how these parameters are estimated and hypotheses tested in the next section.

### 17.2 Linear regression and likelihood

The maximum likelihood method can be used to estimate the parameters for regression models, similar to ANOVA models. Suppose we have $n$ observations conforming to the linear regression model

$$
\begin{equation*}
Y_{i}=\alpha+\beta X_{i}+\epsilon_{i} . \tag{17.2}
\end{equation*}
$$

## Linear regression model



Figure 17.1: The linear regression model plotted across a range of $X$ values, with $\alpha=2.0, \beta=3.0$, and $\sigma^{2}=2.5$.

This model has three parameters to estimate, namely $\alpha, \beta$, and $\sigma^{2}$ (the variance of $\epsilon_{i}$ ). What would the likelihood function be for these data? Consider the first observation in the $D$. frontalis cage experiment, for which $Y_{1}=1.250$ and $X_{1}=0.100$. For this observation, the model states that $Y_{1} \sim N\left(\alpha+\beta X_{1}, \sigma^{2}\right)$, and so the likelihood would be

$$
\begin{equation*}
L_{1}=\frac{1}{\sqrt{2 \pi \sigma^{2}}} e^{-\frac{1}{2} \frac{\left(Y_{1}-\left(\alpha+\beta X_{1}\right)\right)^{2}}{\sigma^{2}}}=\frac{1}{\sqrt{2 \pi \sigma^{2}}} e^{-\frac{1}{2} \frac{(1.250-(\alpha+\beta 0.100))^{2}}{\sigma^{2}}} \tag{17.3}
\end{equation*}
$$

The likelihood $L_{i}$ for the $i t h$ observation would be similar, and the overall likelihood is defined as their product:

$$
\begin{equation*}
L\left(\alpha, \beta, \sigma^{2}\right)=L_{1} \times L_{2} \times \ldots \times L_{n} \tag{17.4}
\end{equation*}
$$

Finding the maximum likelihood estimates involves maximizing this quantity with respect to the parameters $\alpha, \beta$, and $\sigma^{2}$. Using some calculus to find the maximum, it can be shown that estimators of these parameters are

$$
\begin{gather*}
\hat{\beta}=\frac{\sum_{i=1}^{n}\left(Y_{i}-\bar{Y}\right)\left(X_{i}-\bar{X}\right)}{\sum_{i=1}^{n}\left(X_{i}-\bar{X}\right)^{2}},  \tag{17.5}\\
\hat{\alpha}=\bar{Y}-\hat{\beta} \bar{X} \tag{17.6}
\end{gather*}
$$

and

$$
\begin{equation*}
\hat{\sigma}^{2}=\frac{\sum_{i=1}^{n}\left(Y_{i}-\left(\hat{\alpha}+\hat{\beta} X_{i}\right)\right)^{2}}{n-2}=\frac{\sum_{i=1}^{n}\left(Y_{i}-\hat{Y}_{i}\right)^{2}}{n-2} . \tag{17.7}
\end{equation*}
$$

Here $\hat{Y}_{i}=\hat{\alpha}+\hat{\beta} X_{i}$, the value of $Y_{i}$ predicted by the model at $X_{i}$.
We can gain some insight into the estimation process by rearranging the likelihood function. It can be written in the form

$$
\begin{equation*}
L\left(\alpha, \beta, \sigma^{2}\right)=\left(\frac{1}{\sqrt{2 \pi \sigma^{2}}}\right)^{n} e^{-\frac{1}{2} \frac{\sum_{i=1}^{n}\left(Y_{i}-\left(\alpha+\beta X_{i}\right)\right)^{2}}{\sigma^{2}}} . \tag{17.8}
\end{equation*}
$$

Now examine the terms in the sum, which are of the form $\left(Y_{i}-\left(\alpha+\beta X_{i}\right)\right)^{2}$. Values of $\alpha$ and $\beta$ that minimize these terms will make the overall likelihood larger, because of the negative sign in the exponent. The likelihood will reach its maximum when this sum is smallest. Thus, values of $\alpha$ and $\beta$ that minimize

$$
\begin{equation*}
\sum_{i=1}^{n}\left(Y_{i}-\left(\alpha+\beta X_{i}\right)\right)^{2} \tag{17.9}
\end{equation*}
$$

are the maximum likelihood estimates. These estimates are also called least squares estimates because they minimize the sum of these squared terms. In fact, we could directly estimate $\alpha$ and $\beta$ using this method without recourse to likelihood (Searle 1971). The two methods yield the same results when the data have a normal distribution.

A likelihood ratio test for linear regression can be constructed as follows. Suppose we want to test $H_{0}: \beta=0$ vs. $H_{1}: \beta \neq 0$, the latter implying a linear relationship between $Y$ and $X$. The statistical model under $H_{0}$ would be

$$
\begin{align*}
Y_{i} & =\alpha+\beta X_{i}+\epsilon_{i}  \tag{17.10}\\
& =\alpha+\epsilon_{i} \tag{17.11}
\end{align*}
$$

because $\beta=0$ under $H_{0}$. The statistical model under $H_{1}$ would be the full model including a slope term, namely

$$
\begin{equation*}
Y_{i}=\alpha+\beta X_{i}+\epsilon_{i} \tag{17.12}
\end{equation*}
$$

We would need to find the maximum likelihood estimates under both $H_{1}$ (see previous section) and $H_{0}$, as well as $L_{H_{0}}$ and $L_{H_{1}}$, the maximum height of
the likelihood function under $H_{0}$ and $H_{1}$. We would then use the likelihood ratio test statistic

$$
\begin{equation*}
\lambda=\frac{L_{H_{0}}}{L_{H_{1}}} \tag{17.13}
\end{equation*}
$$

There is a one-to-one correspondence between $-2 \ln (\lambda)$ and the statistic $F_{s}$ used to test this null hypothesis (McCulloch \& Searle 2001).

We can gain further insight into this test by defining various sum of squares and mean squares used to calculate $F_{s}$. In particular, we will define $S S_{\text {error }}, S S_{\text {regression }}$, and $S S_{\text {total }}$ and their associated mean squares, which have functions similar to those in ANOVA. We will also summarize the calculations in an ANOVA table.
$S S_{\text {error }}$ describes variation in the data around the regression line, or variation not explained by the model. It is defined as

$$
\begin{equation*}
S S_{\text {error }}=\sum_{i=1}^{n}\left(Y_{i}-\left(\hat{\alpha}+\hat{\beta} X_{i}\right)\right)^{2}=\sum_{i=1}^{n}\left(Y_{i}-\hat{Y}_{i}\right)^{2} \tag{17.14}
\end{equation*}
$$

$S S_{\text {error }}$ has $n-2$ degrees of freedom. We can therefore define

$$
\begin{equation*}
M S_{\text {error }}=\frac{S S_{\text {error }}}{n-2}=\hat{\sigma}^{2} \tag{17.15}
\end{equation*}
$$

Thus, $M S_{\text {error }}$ is equivalent to $\hat{\sigma}^{2}$, the maximum likelihood estimate of $\sigma^{2}$, the same relationship as found in ANOVA. $S S_{\text {error }}$ and $M S_{\text {error }}$ will be small if the data lie on a straight line and large if the data are scattered around the line.
$S S_{\text {regression }}$ describes variation in the data explained by the regression model. It is defined as

$$
\begin{equation*}
S S_{\text {regression }}=\sum_{i=1}^{n}\left(\hat{Y}_{i}-\bar{Y}\right)^{2} \tag{17.16}
\end{equation*}
$$

and has one degree of freedom. We therefore have

$$
\begin{equation*}
M S_{\text {regression }}=\frac{S S_{\text {regression }}}{1}=S S_{\text {regression }} \tag{17.17}
\end{equation*}
$$

$S S_{\text {regression }}$ and $M S_{\text {regression }}$ will be large if the data have a strong positive or negative slope. To see this, recall that $\hat{Y}_{i}=\hat{\alpha}+\hat{\beta} X_{i}$. If the estimated slope
$\hat{\beta}$ is large, the values of $\hat{Y}_{i}$ will vary strongly as $X_{i}$ changes and so generate a large sum of squares.

The total sum of squares is defined (as in ANOVA) to be

$$
\begin{equation*}
S S_{\text {total }}=\sum_{i=1}^{n}\left(Y_{i}-\bar{Y}\right)^{2} \tag{17.18}
\end{equation*}
$$

and has $n-1$ degrees of freedom. There is also a familiar relationship among the different sums of squares, namely

$$
\begin{equation*}
S S_{\text {regression }}+S S_{\text {error }}=S S_{\text {total }} . \tag{17.19}
\end{equation*}
$$

The likelihood ratio statistic used to test $H_{0}: \beta=0$ is defined as

$$
\begin{equation*}
F_{s}=\frac{M S_{\text {regression }}}{M S_{\text {error }}} . \tag{17.20}
\end{equation*}
$$

Under $H_{0}, F_{s}$ has an $F$ distribution with $d f_{1}=1$ and $d f_{2}=n-2$ the degrees of freedom. Given the definitions of $M S_{\text {regression }}$ and $M S_{\text {error }}$, we can see that $F_{s}$ tends to be large when the data have a strong slope (the numerator of this expression) relative to the amount of scatter in the data (the denominator).

We can organize the different sum of squares and mean squares into an ANOVA table for linear regression. It lists the different sources of variation in the data (regression, error, and total), their degrees of freedom, as well as the $F$ test. Table 17.2 shows the general layout for linear regression.

Table 17.2: General ANOVA table for linear regression, showing formulas for different mean squares and the $F$ test.

| Source | $d f$ | Sum of squares | Mean square | $F_{s}$ |
| :--- | :---: | :---: | :---: | :---: |
| Regression | 1 | $S S_{\text {regression }}$ | $M S_{\text {regression }}=S S_{\text {regression }} / 1$ | $M S_{\text {regression }} / M S_{\text {error }}$ |
| Error | $n-2$ | $S S_{\text {error }}$ | $M S_{\text {error }}=S S_{\text {error }} /(n-2)$ |  |
| Total | $n-1$ | $S S_{\text {total }}$ |  |  |

Table 17.3: ANOVA table for the Example 1 data set, including a $P$ value for the test.

| Source | $d f$ | Sum of squares | Mean square | $F_{s}$ | $P$ |
| :--- | :---: | ---: | ---: | ---: | :---: |
| Regression | 1 | 82.528 | 82.528 | 32.504 | $<0.001$ |
| Error | 25 | 63.486 | 2.539 |  |  |
| Total | 26 | 146.014 |  |  |  |

### 17.2.1 Sample calculation $-\hat{\beta}, \hat{\alpha}$, and $F$ test

We will illustrate the above calculations using the Example 1 data set, where $Y$ is $D$. frontalis attack density and $X$ is the number of beetles added to the cage. We are interested in estimating the slope and intercept ( $\beta$ and $\alpha$ ) of the relationship between the two variables, and then testing whether the slope is significantly different from zero $\left(H_{0}: \beta=0\right)$.

The first step is to calculate the sample mean for both $Y$ and $X$, and we obtain $\bar{Y}=4.481$ and $\bar{X}=0.960$. We then calculate $\left(X_{i}-\bar{X}\right)^{2}$ for each value of $X_{i}$ (see Table 17.1) and sum these values to obtain

$$
\begin{equation*}
\sum_{i=1}^{n}\left(X_{i}-\bar{X}\right)^{2}=11.798 \tag{17.21}
\end{equation*}
$$

We then calculate $\left(Y_{i}-\bar{Y}\right)\left(X_{i}-\bar{X}\right)$ for each pair of numbers and sum these to obtain

$$
\begin{equation*}
\sum_{i=1}^{n}\left(Y_{i}-\bar{Y}\right)\left(X_{i}-\bar{X}\right)=31.203 \tag{17.22}
\end{equation*}
$$

The estimate of $\beta$ can then be calculated, and we find

$$
\begin{equation*}
\hat{\beta}=\frac{\sum_{i=1}^{n}\left(Y_{i}-\bar{Y}\right)\left(X_{i}-\bar{X}\right)}{\sum_{i=1}^{n}\left(X_{i}-\bar{X}\right)^{2}}=\frac{31.203}{11.798}=2.645 \tag{17.23}
\end{equation*}
$$

We can then estimate $\alpha$ using the formula

$$
\begin{equation*}
\hat{\alpha}=\bar{Y}-\hat{\beta} \bar{X}=4.481-2.645(0.960)=1.942 \tag{17.24}
\end{equation*}
$$

The next step is to calculate the predicted values of $Y_{i}$ using the formula $\hat{Y}_{i}=\hat{\alpha}+\hat{\beta} X_{i}$, for each value of $X_{i}$ (see Table 17.1). We then calculate $Y_{i}-\hat{Y}_{i}$ in another column - these are the residuals for each observation. Squaring and summing the residuals, we find

$$
\begin{equation*}
S S_{\text {error }}=\sum_{i=1}^{n}\left(Y_{i}-\hat{Y}_{i}\right)^{2}=63.486, \tag{17.25}
\end{equation*}
$$

and

$$
\begin{equation*}
M S_{\text {error }}=\frac{S S_{\text {error }}}{n-2}=\frac{63.486}{27-2}=2.539 . \tag{17.26}
\end{equation*}
$$

We next calculate a column consisting of $\left(\hat{Y}_{i}-\bar{Y}\right)^{2}$ for each observation, then sum these values to obtain

$$
\begin{equation*}
S S_{\text {regression }}=\sum_{i=1}^{n}\left(\hat{Y}_{i}-\bar{Y}\right)^{2}=82.528 \tag{17.27}
\end{equation*}
$$

and so

$$
\begin{equation*}
M S_{\text {regression }}=S S_{\text {regression }} / 1=82.528 \tag{17.28}
\end{equation*}
$$

We are now in a position to calculate $F_{s}$, the statistic used to test $H_{0}$ : $\beta=0$. We have

$$
\begin{equation*}
F_{s}=\frac{M S_{\text {regression }}}{M S_{\text {error }}}=\frac{82.528}{2.539}=32.504 \tag{17.29}
\end{equation*}
$$

Under $H_{0}, F_{s}$ has an $F$ distribution with $d f_{1}=1$ and $d f_{2}=27-2=25$ degrees of freedom. Using Table F, we find the $P<0.001$. There was a highly significant effect of beetles numbers on the attack density of $D$. frontalis $\left(F_{1,25}=32.504, P<0.001\right)$.

The last column in Table 17.1 calculates $\left(Y_{i}-\bar{Y}\right)^{2}$, the components of $S S_{\text {total }}$. Summing these components we obtain $S S_{\text {total }}=146.014$. It can also be calculated using the formula $S S_{\text {regression }}+S S_{\text {error }}=S S_{\text {total }}$. Table 17.3 shows the completed ANOVA table.

The observations for Example 1 and the fitted linear regression model are shown in Fig. 17.2. The estimation procedure (maximum likelihood or least squares) finds values of $\alpha$ and $\beta$ that minimize the sum of the squared differences between the data points and the line. In particular, it minimizes the sum of the squared residuals, where the residuals are $Y_{i}-\hat{Y}_{i}=Y_{i}-(\hat{\alpha}+$ $\hat{\beta} X_{i}$ ).


Figure 17.2: Linear regression model fitted to the Example 1 data, where $Y$ is attack density and $X$ is beetles added to the cages. The vertical dashed line shows the residual $Y_{4}-\hat{Y}_{4}=-3.648$ for the $i=4$ observation.

### 17.3 Confidence and prediction intervals

In this section, we will derive confidence intervals for the parameters of the regression model ( $\alpha$ and $\beta$ ) that provide a measure of their precision (see Chapter 9). We will also find confidence intervals for the mean value of $Y_{i}$ at a given value of $X_{i}$. Another type of interval for linear regression are prediction intervals. These are used to set limits for future $Y_{i}$ values given some value of $X_{i}$. Both of these intervals are used in prediction, another common purpose for linear regression. See Draper \& Smith (1981) for further details.

The confidence interval for the slope $\beta$ is based on $\hat{\beta}$, the maximum likelihood estimate of $\beta$, and the standard error of this estimate $s_{\hat{\beta}}$, given by the formula

$$
\begin{equation*}
s_{\hat{\beta}}=\sqrt{\frac{\hat{\sigma}^{2}}{\sum_{i=1}^{n}\left(X_{i}-\bar{X}\right)^{2}}} \tag{17.30}
\end{equation*}
$$

where $\hat{\sigma}^{2}=M S_{\text {error }}$. Note that $s_{\hat{\beta}}$ depends on the scatter of the data around the line $\left(\hat{\sigma}^{2}\right)$ as well as the amount of variability in $X_{i}$. A study using a larger range of $X_{i}$ values will thus provide a more precise estimate of $\beta$, because it reduces $s_{\hat{\beta}}$. Increasing the sample size $n$ would also increase the precision, by increasing the sum of squares in the denominator for $s_{\hat{\beta}}$.

It can be shown that the quantity

$$
\begin{equation*}
\frac{\hat{\beta}-\beta}{s_{\hat{\beta}}} \tag{17.31}
\end{equation*}
$$

has a $t$ distribution with $n-2$ degrees of freedom, the same as for $M S_{\text {error }}$. This fact can be used to derive a confidence interval for $\beta$. Using Table T, we first find a value of $c_{\alpha, n-2}$ for $n-2$ degrees of freedom such that the following equation is true:

$$
\begin{equation*}
P\left[-c_{\alpha, n-2}<\frac{\hat{\beta}-\beta}{s_{\hat{\beta}}}<c_{\alpha, n-2}\right]=1-\alpha . \tag{17.32}
\end{equation*}
$$

Rearranging this equation we obtain

$$
\begin{equation*}
P\left[\hat{\beta}-c_{\alpha, n-2} s_{\hat{\beta}}<\beta<\hat{\beta}+c_{\alpha, n-2} s_{\hat{\beta}}\right]=1-\alpha . \tag{17.33}
\end{equation*}
$$

It follows that the interval

$$
\begin{equation*}
\left(\hat{\beta}-c_{\alpha, n-2} s_{\hat{\beta}}, \hat{\beta}+c_{\alpha, n-2} s_{\hat{\beta}}\right) \tag{17.34}
\end{equation*}
$$

is a $100(1-\alpha) \%$ confidence interval for $\beta$. The center of the confidence interval would be $\hat{\beta}$.

We may also want to test various null hypotheses concerning $\beta$. For example, we may want to test $H_{0}: \beta=\beta_{0}$ vs. $H_{1}: \beta \neq \beta_{0}$, where $\beta_{0}$ takes some value of interest. Similar to the approach in Chapter 10, we would use the test statistic

$$
\begin{equation*}
T_{s}=\frac{\hat{\beta}-\beta_{0}}{s_{\hat{\beta}}} . \tag{17.35}
\end{equation*}
$$

Under $H_{0}, T_{s}$ has a $t$ distribution with $n-2$ degrees of freedom, and we would reject $H_{0}$ for sufficiently large values of this statistic. For $\beta_{0}=0$, this test is equivalent to the $F$ test we developed earlier for $H_{0}: \beta=0$, and in fact $T_{s}^{2}=F_{s}$. The $t$ test is more general, however, because we can also test $H_{0}: \beta=\beta_{0}$ for any value of $\beta_{0}$.

It is possible to derive similar $t$ tests and confidence intervals for the intercept parameter $\alpha$. The $t$ test is most commonly used to test $H_{0}: \alpha=0$. If the test is significant this implies an intercept different from zero. We will let SAS handle the calculations here.

We can also derive a confidence interval for the theoretical mean of $Y_{i}$ at a given $X_{i}$ value. Recall that according to the linear regression model, $E\left[Y_{i}\right]=\alpha+\beta X_{i}$. Thus, $Y_{i}$ has a mean of $\mu_{i}=\alpha+\beta X_{i}$ for any $X_{i}$ value. The confidence interval is based on $\hat{Y}_{i}=\hat{\alpha}+\hat{\beta} X_{i}$, the predicted value of $Y_{i}$ at $X_{i}$. It also depends on the standard error $s_{\hat{Y}}$ of $\hat{Y}$, which is given by the formula

$$
\begin{equation*}
s_{\hat{Y}}=\sqrt{\hat{\sigma}^{2}\left[\frac{1}{n}+\frac{\left(X_{i}-\bar{X}\right)^{2}}{\sum_{i=1}^{n}\left(X_{i}-\bar{X}\right)^{2}}\right]} . \tag{17.36}
\end{equation*}
$$

Note that the standard error $s_{\hat{Y}}$ depends on the value of $\left(X_{i}-\bar{X}\right)^{2}$, which is the squared distance of $X_{i}$ from $\bar{X}$. The farther $X_{i}$ is from $\bar{X}$, the larger the value of $s_{\hat{Y}}$.

Using methods similar to the confidence interval for $\beta$, it can be shown that a $100(1-\alpha)$ confidence interval for $\mu_{i}=\alpha+\beta X_{i}$ has the form

$$
\begin{equation*}
\left(\hat{Y}_{i}-c_{\alpha, n-2} s_{\hat{Y}}, \hat{Y}_{i}+c_{\alpha, n-2} s_{\hat{Y}}\right) \tag{17.37}
\end{equation*}
$$

The interval will be broader for values of $X_{i}$ far from $\bar{X}$ because $s_{\hat{Y}}$ will be larger. In other words, the precision of the confidence interval decreases with the distance from $\bar{X}$.

We next examine prediction intervals. Here, we are trying to find an interval that contains a defined percentage of future $Y_{i}$ values for a given value of $X_{i}$. These are similar in form to the intervals for the theoretical mean $\mu_{i}=\alpha+\beta X_{i}$, but are always wider because you are trying to enclose a single future observation rather than a mean value.

The prediction interval is based on $\hat{Y}_{i}=\hat{\alpha}+\hat{\beta} X_{i}$, the predicted value of $Y_{i}$ at $X_{i}$, and the standard error $s_{\hat{Y}(1)}$ of $\hat{Y}_{i}$, which is given by the formula

$$
\begin{equation*}
s_{\hat{Y}(1)}=\sqrt{\hat{\sigma}^{2}\left[1+\frac{1}{n}+\frac{\left(X_{i}-\bar{X}\right)^{2}}{\sum_{i=1}^{n}\left(X_{i}-\bar{X}\right)^{2}}\right]} . \tag{17.38}
\end{equation*}
$$

Note the additional term (1+) within the square brackets, which makes this standard error larger than $s_{\hat{Y}}$. It also depends on the value of $\left(X_{i}-\bar{X}\right)^{2}$, and so the farther $X_{i}$ is from $\bar{X}$, the larger the value of $s_{\hat{Y}(1)}$. It can be shown that a $100(1-\alpha)$ prediction interval for a single future $Y_{i}$ has the form

$$
\begin{equation*}
\left(\hat{Y}_{i}-c_{\alpha, n-2} s_{\hat{Y}(1)}, \hat{Y}_{i}+c_{\alpha, n-2} s_{\hat{Y}(1)}\right) \tag{17.39}
\end{equation*}
$$

### 17.3.1 Sample calculation - confidence and prediction intervals

We now illustrate the calculations for confidence intervals using the Example 1 data. We earlier found that $\hat{\beta}=2.645$ and $\hat{\alpha}=1.942$. To find a confidence interval for $\beta$, we first need to calculate $s_{\hat{\beta}}$. From Table 17.1, we see that $\sum_{i=1}^{n}\left(X_{i}-\bar{X}\right)^{2}=11.798$, and we earlier calculated that $\hat{\sigma}^{2}=M S_{\text {error }}=$ 2.539. Inserting these quantities into the formula for $s_{\hat{\beta}}$, we find

$$
\begin{equation*}
s_{\hat{\beta}}=\sqrt{\frac{\hat{\sigma}^{2}}{\sum_{i=1}^{n}\left(X_{i}-\bar{X}\right)^{2}}}=\sqrt{\frac{2.539}{11.798}}=0.464 \tag{17.40}
\end{equation*}
$$

A $95 \%$ confidence interval for $\beta$ has the form

$$
\begin{equation*}
\left(\hat{\beta}-c_{0.05, n-2} s_{\hat{\beta}}, \hat{\beta}+c_{0.05, n-2} s_{\hat{\beta}}\right) \tag{17.41}
\end{equation*}
$$

From Table T with $d f=n-2=27-2=25$, we find that $c_{0.05,25}=2.060$. Inserting this value, $\hat{\beta}=2.645$, and $s_{\hat{\beta}}=0.464$ in the above formula, we obtain

$$
\begin{equation*}
(2.645-2.060(0.464), 2.645+2.060(0.464)) \tag{17.42}
\end{equation*}
$$

or

$$
\begin{equation*}
(1.689,3.601) \tag{17.43}
\end{equation*}
$$

We next find a confidence interval for the theoretical mean $\mu_{i}=\alpha+\beta X_{i}$ at $X_{i}=1.75$. We first need to find the predicted value $\hat{Y}_{i}$ for this value of $X_{i}$, using the estimated intercept and slope. We have

$$
\begin{equation*}
\hat{Y}_{i}=\hat{\alpha}+\hat{\beta} X_{i}=1.942+2.645(1.75)=6.571 \tag{17.44}
\end{equation*}
$$

The standard error $s_{\hat{Y}}$ for this interval also uses $\sum_{i=1}^{n}\left(X_{i}-\bar{X}\right)^{2}=11.798$ and $\hat{\sigma}^{2}=2.539$, and we earlier found that $\bar{X}=0.960$. Inserting these quantities into the formula for $s_{\hat{Y}}$, we find that

$$
\begin{align*}
s_{\hat{Y}} & =\sqrt{\hat{\sigma}^{2}\left[\frac{1}{n}+\frac{\left(X_{i}-\bar{X}\right)^{2}}{\sum_{i=1}^{n}\left(X_{i}-\bar{X}\right)^{2}}\right]}  \tag{17.45}\\
& =\sqrt{2.539\left[\frac{1}{27}+\frac{(1.75-0.960)^{2}}{11.798}\right]}  \tag{17.46}\\
& =\sqrt{2.539\left[0.037+\frac{0.624}{11.798}\right]}  \tag{17.47}\\
& =0.478 . \tag{17.48}
\end{align*}
$$

A $95 \%$ confidence interval for the theoretical mean $\mu_{i}=\alpha+\beta X_{i}$ has the form

$$
\begin{equation*}
\left(\hat{Y}-c_{0.05, n-2} s_{\hat{Y}}, \hat{Y}+c_{0.05, n-2} s_{\hat{Y}}\right) \tag{17.49}
\end{equation*}
$$

Inserting $\hat{Y}=6.571, s_{\hat{Y}}=0.478$, and $c_{0.05,25}=2.060$ in the above formula, we find

$$
\begin{equation*}
(6.571-2.060(0.478), 6.571+2.060(0.478)) \tag{17.50}
\end{equation*}
$$

or

$$
\begin{equation*}
(5.586,7.556) \tag{17.51}
\end{equation*}
$$

Lastly, we calculate a prediction interval for a single future observation $Y_{i}$ at $X_{i}=1.75$. We earlier calculated that $\hat{Y}_{i}=6.571$ for this value of $X_{i}$, and
will again make use of $\sum_{i=1}^{n}\left(X_{i}-\bar{X}\right)^{2}=11.798, \bar{X}=0.960$ and $\hat{\sigma}^{2}=2.539$. Inserting these quantities into the formula for $s_{\hat{Y}(1)}$, we obtain

$$
\begin{align*}
s_{\hat{Y}(1)} & =\sqrt{\hat{\sigma}^{2}\left[1+\frac{1}{n}+\frac{\left(X_{i}-\bar{X}\right)^{2}}{\sum_{i=1}^{n}\left(X_{i}-\bar{X}\right)^{2}}\right]}  \tag{17.52}\\
& =\sqrt{2.539\left[1+\frac{1}{27}+\frac{(1.75-0.960)^{2}}{11.798}\right]}  \tag{17.53}\\
& =\sqrt{2.539\left[1+0.037+\frac{0.624}{11.798}\right]}  \tag{17.54}\\
& =1.663 . \tag{17.55}
\end{align*}
$$

A $95 \%$ prediction interval for a single $Y_{i}$ has the form

$$
\begin{equation*}
\left(\hat{Y}-c_{0.05, n-2} s_{\hat{Y}(1)}, \hat{Y}+c_{0.05, n-2} s_{\hat{Y}(1)}\right) \tag{17.56}
\end{equation*}
$$

Inserting $\hat{Y}=6.571, s_{\hat{Y}(1)}=1.663$, and $c_{0.05,25}=2.060$ in this formula, we obtain

$$
\begin{equation*}
(6.571-2.060(1.663), 6.571+2.060(1.663)) \tag{17.57}
\end{equation*}
$$

or

$$
\begin{equation*}
(3.145,9.997) . \tag{17.58}
\end{equation*}
$$

Note this interval is much wider than the interval for the theoretical mean $\mu_{i}=\alpha+\beta X_{i}$, which was $(5.586,7.556)$. This is because you are trying to enclose a single future observation, a random variable $Y_{i}$, rather than a theoretical mean.

## 17.4 $R^{2}$ values

$R^{2}$ values are a measure of how well a statistical model explains the data. Recall that the following relationship holds among the sum of squares in linear regression:

$$
\begin{equation*}
S S_{\text {regression }}+S S_{\text {error }}=S S_{\text {total }} . \tag{17.59}
\end{equation*}
$$

We can think of the different sum of squares as partitioning the variability in the data into different sources. $S S_{\text {regression }}$ represents variability explained by the regression line, $S S_{\text {error }}$ represents variability of the observations around
the regression line, while $S S_{\text {total }}$ is the total amount of variability in the data. The $R^{2}$ value for a linear regression model is the proportion of total variability explained by the model, or

$$
\begin{equation*}
R^{2}=\frac{S S_{\text {regression }}}{S S_{\text {total }}}=\frac{S S_{\text {regression }}}{S S_{\text {regression }}+S S_{\text {error }}} \tag{17.60}
\end{equation*}
$$

It is clear from this formula that $R^{2}$ must range between 0 and $1\left(0 \leq R^{2} \leq\right.$ 1). For the Example 1 data, we have

$$
\begin{equation*}
R^{2}=82.528 / 146.014=0.565 \tag{17.61}
\end{equation*}
$$

Thus, $56.5 \%$ of the variation is explained by the regression model for these data. Small $R^{2}$ values indicate there is substantial variability in the data not explained by the model, while large ones indicate the model explains most of the variation.

More generally, we can define an $R^{2}$ value for both ANOVA and regression models as

$$
\begin{equation*}
R^{2}=\frac{S S_{\text {model }}}{S S_{\text {total }}}=\frac{S S_{\text {model }}}{S S_{\text {model }}+S S_{\text {error }}} \tag{17.62}
\end{equation*}
$$

For example, we have $S S_{\text {model }}=S S_{\text {among }}$ for one-way ANOVA while $S S_{\text {error }}=$ $S S_{\text {within. }}$. The $R^{2}$ value here is the proportion of the variation explained by the one-way ANOVA model, in particular the variation among the group means. The SAS output for proc glm provides an $R^{2}$ for ANOVA models of this form.

### 17.5 Linear regression for Example 1 - SAS demo

The linear regression analysis can be conducted using proc glm and a program similar in structure to ANOVA ones (see SAS program below). We first input the observations using a data step, with the first variable standing for attack density (attacks) while the second is the number of beetles added (beetles). The next two lines in the data step define which of these two variables are the dependent and independent ones. The line y $=$ attacks sets attack density as the dependent variable, while $\mathrm{x}=$ beetles is the independent variable. The remainder of the program then uses $y$ and $x$ rather than the original variables
and so does not need to be changed for other data sets. Transformations of the observations could also be applied at this point.

Note the additional observation at end of the data set, for which beetles is 1.75 but attacks is a missing value. The purpose is to make proc glm calculate confidence and prediction intervals for attack density for that particular number of beetles.

The data are then plotted along with the fitted line plus confidence and prediction intervals. This accomplished using the following proc gplot code (SAS Institute Inc. 2016). The three $\mathrm{y} * \mathrm{x}$ statements in the plot command plot the same data in three different ways, which are then combined into one graph using the overlay option. The first plot, using the symboll command, draws the data points. The second plot, using the symbol2 command, draws a regression line through the points and also plots $95 \%$ confidence intervals for the mean of $Y_{i}$ at $X_{i}$, or $\mu_{i}=\alpha+\beta X_{i}$, across the range of $X_{i}$ values. The third plot, using the symbol3 command, plots $95 \%$ prediction intervals for a single future observation, again across the range of $X_{i}$ values. A similar plot is also generated by proc glm for linear regression models (see Fig. 17.9).

The regression analysis is conducted using proc glm as shown below (SAS Institute Inc. 2018). There is no class statement because the independent variable x is a continuous variable and does not fall into discrete groups as with ANOVA. Note the similarity of the model statement to the linear regression model. The option clparm is used to generate $95 \%$ confidence intervals for $\alpha$ and $\beta$, while clm generates a $95 \%$ confidence interval for the mean of $Y_{i}$ at each value of $X_{i}$. If we want prediction intervals it is necessary to run proc glm a second time using the cli option in the model statement (see below). This is necessary because proc glm cannot generate both types of intervals at the same time.

The data points, regression line, and confidence or prediction intervals are shown in Fig. 17.4. The prediction intervals are much wider than the confidence intervals, because the prediction intervals are for single future $Y_{i}$ while the confidence intervals enclose a mean. Note that both types of interval increase in width as you move away from the center of the $X$ values. This follows from the fact that the standard errors involved in these calculations are a function of $\left(X_{i}-\bar{X}\right)^{2}$, which increases as $X_{i}$ moves away from $\bar{X}$.

Examining the output for proc glm, first note that the slope $\beta$ is labeled as x while the intercept $\alpha$ is Intercept (Fig. 17.5). We see that attack density y increases with beetle numbers x , because $\hat{\beta}=2.645$ and is positive. The effect of beetle numbers on attack density was highly significant $\left(F_{1,25}=\right.$
$32.5, P<0.0001)$. There are several $F$ tests to chose from in the output, but all give the same result for simple linear regression. Alternately, we could report the $t$ test for $\beta\left(t_{25}=5.70, P<0.0001\right)$, which also tests $H_{0}: \beta=0$. We see that $R^{2}=0.565$, indicating that $56.5 \%$ of the variation is explained by the regression model.

The proc glm output also provides $95 \%$ confidence intervals for $\alpha$ and $\beta$. A $95 \%$ confidence interval for the mean of $Y_{i}$ at each $X_{i}$ value is also given (Fig. 17.6), as well as $95 \%$ prediction intervals for a single future $Y_{i}$ (Fig. 17.7). These intervals were also calculated for $X_{i}=1.75$ and match our earlier results.

Note that the estimated intercept is some distance from zero $(\hat{\alpha}=1.942)$, and in fact the $t$ test of $H_{0}: \alpha=0$ reported by SAS was highly significant $\left(t_{25}=3.59, P=0.0014\right)$. This cannot really be true because the addition of zero beetles should give you an attack density of zero. A more resonable (and possibly non-linear) model would require that the intercept be zero. This is a potential pitfall when using linear regression. Many biological phenomenon are approximately linear over some range of the data but the approximation breaks down for more extreme values. A linear regression does not take this possibility into account and so cannot provide a general explanation of some phenomena.

## SAS Program

```
* SPBattack2.sas;
title 'Linear regression for D. frontalis attack density';
data frontalis;
    input attacks beetles;
    * Apply transformations here;
    y = attacks;
    x = beetles;
    datalines;
1.25 0.100
2.66 1.000
7.33 2.000
1.60 1.250
2.62 0.500
etc.
5.00 0.500
. 1.750
;
run;
* Print data set;
proc print data=frontalis;
run;
* Plot data and regression line;
proc gplot data=frontalis;
    plot y*x y*x y*x / overlay vaxis=axis1 haxis=axis1;
    symbol1 i=none v=star c=black height=2 width=3;
    symbol2 i=rlclm v=none c=red height=2 width=3;
    symbol3 i=rlcli v=none c=blue height=2 width=3;
    axis1 label=(height=2) value=(height=2) width=3 major=(width=2) minor=none;
run;
* Regression analysis with confidence intervals;
proc glm plots=diagnostics data=frontalis;
    model y = x / clparm clm;
run;
* Regression analysis with prediction intervals;
proc glm data=frontalis;
    model y = x / clparm cli;
run;
quit;
```


## Linear regression for D. frontalis attack density

| Obs | attacks | beetles | $\mathbf{y}$ | $\mathbf{x}$ |
| ---: | ---: | ---: | ---: | ---: |
| $\mathbf{1}$ | 1.25 | 0.100 | 1.25 | 0.100 |
| $\mathbf{2}$ | 2.66 | 1.000 | 2.66 | 1.000 |
| $\mathbf{3}$ | 7.33 | 2.000 | 7.33 | 2.000 |
| $\mathbf{4}$ | 1.60 | 1.250 | 1.60 | 1.250 |
| $\mathbf{5}$ | 2.62 | 0.500 | 2.62 | 0.500 |
| $\mathbf{6}$ | 1.00 | 0.200 | 1.00 | 0.200 |
| $\mathbf{7}$ | 4.34 | 1.500 | 4.34 | 1.500 |
| $\mathbf{8}$ | 5.23 | 0.750 | 5.23 | 0.750 |
| $\mathbf{9}$ | 2.50 | 0.250 | 2.50 | 0.250 |
| $\mathbf{1 0}$ | 3.25 | 0.500 | 3.25 | 0.500 |

Figure 17.3: SPBattack.sas - proc print


Figure 17.4: SPBattack.sas - proc gplot

# Linear regression for D. frontalis attack density The GLM Procedure 

Number of Observations Read 28<br>Number of Observations Used 27

Linear regression for D. frontalis attack density
The GLM Procedure
Dependent Variable: y

| Source | DF | Sum of Squares | Mean Square | F Value | Pr > F |
| :--- | ---: | ---: | ---: | ---: | ---: |
| Model | 1 | 82.5283492 | 82.5283492 | 32.50 | $<.0001$ |
| Error | 25 | 63.4855174 | 2.5394207 |  |  |
| Corrected Total | 26 | 146.0138667 |  |  |  |


| R-Square | Coeff Var | Root MSE | y Mean |
| ---: | ---: | ---: | ---: |
| 0.565209 | 35.56163 | 1.593556 | 4.481111 |


| Source | DF | Type I SS | Mean Square | F Value | Pr > F |
| :--- | ---: | ---: | ---: | ---: | ---: |
| $\mathbf{x}$ | 1 | 82.52834922 | 82.52834922 | 32.50 | $<.0001$ |


| Source | DF | Type III SS | Mean Square | F Value | Pr > F |
| :--- | ---: | ---: | ---: | ---: | ---: |
| $\mathbf{x}$ | 1 | 82.52834922 | 82.52834922 | 32.50 | $<.0001$ |


| Parameter | Estimate | Standard <br> Error | $\mathbf{t}$ Value | $\operatorname{Pr}>\|\mathbf{t}\|$ | 95\% Confidence Limits |  |
| :--- | ---: | ---: | ---: | ---: | ---: | ---: |
| Intercept | 1.941567811 | 0.54083158 | 3.59 | 0.0014 | 0.827704323 | 3.055431300 |
| $\mathbf{x}$ | 2.644847410 | 0.46394486 | 5.70 | $<.0001$ | 1.689335080 | 3.600359740 |

Figure 17.5: SPBattack.sas - proc glm

## Linear regression for D. frontalis attack density

## The GLM Procedure

| Observation | Observed | Predicted | Residual | 95\% Confidence Limits for | icted Value |
| :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 1.25000000 | 2.20605255 | -0.95605255 | 1.16947580 | 3.24262930 |
| 2 | 2.66000000 | 4.58641522 | -1.92641522 | 3.95365127 | 5.21917917 |
| 3 | 7.33000000 | 7.23126263 | 0.09873737 | 6.05393677 | 8.40858849 |
| 4 | 1.60000000 | 5.24762707 | -3.64762707 | 4.55796883 | 5.93728532 |
| 5 | 2.62000000 | 3.26399152 | -0.64399152 | 2.49438766 | 4.03359537 |
| etc. |  |  |  |  |  |
| 24 | 4.75000000 | 4.58641522 | 0.16358478 | 3.95365127 | 5.21917917 |
| 25 | 4.50000000 | 2.60277966 | 1.89722034 | 1.67572614 | 3.52983319 |
| 26 | 9.56000000 | 7.23126263 | 2.32873737 | 6.05393677 | 8.40858849 |
| 27 | 5.00000000 | 3.26399152 | 1.73600848 | 2.49438766 | 4.03359537 |
| 28 |  | 6.57005078 |  | 5.58593621 | 7.55416534 |

Figure 17.6: SPBattack.sas - proc glm

Linear regression for D. frontalis attack density
The GLM Procedure

| Observation | Observed | Predicted | Residual | 95\% Confidence Limits for Individual Predicted Value |  |
| ---: | ---: | ---: | ---: | ---: | ---: |
| $\mathbf{1}$ | 1.25000000 | 2.20605255 | -0.95605255 | -1.23574200 | 5.64784710 |
| $\mathbf{2}$ | 2.66000000 | 4.58641522 | -1.92641522 | 1.24398368 | 7.92884676 |
| $\mathbf{3}$ | 7.33000000 | 7.23126263 | 0.09873737 | 3.74449413 | 10.71803113 |
| $\mathbf{4}$ | 1.60000000 | 5.24762707 | -3.64762707 | 1.89395940 | 8.60129475 |
| $\mathbf{5}$ | 2.62000000 | 3.26399152 | -0.64399152 | -0.10702442 | 6.63500745 |
|  |  |  | etc. |  |  |
| $\mathbf{2 4}$ | 4.75000000 | 4.58641522 | 0.16358478 |  |  |
| $\mathbf{2 5}$ | 4.50000000 | 2.60277966 | 1.89722034 | 1.24398368 | 6.92884676 |
| $\mathbf{2 6}$ | 9.56000000 | 7.23126263 | 2.32873737 | -0.80762891 | 6.01318823 |
| $\mathbf{2 7}$ | 5.00000000 | 3.26399152 | 1.73600848 | 3.74449413 | 10.71803113 |
| $\mathbf{2 8}$ | $*$ | . | 6.57005078 | -0.10702442 | 6.63500745 |
|  |  |  | 3.14369122 | 9.99641034 |  |

Figure 17.7: SPBattack.sas - proc glm


Figure 17.8: SPBattack.sas - proc glm


Figure 17.9: SPBattack.sas - proc glm

### 17.6 Assumptions and transformations

Linear regression makes the same assumptions as ANOVA, including homogeneity of variances and normality, and the same types of plots can be used to assess them. If the homogeneity of variances assumption is satisfied, the points in a residual vs. predicted plot should be equally scattered across the range of predicted values. Outliers can also be identified using this plot. The normality assumption can be evaluated using a normal quantile plot of the residuals, with a straight diagonal line indicating this assumption is satisfied.

Examining the residuals from the Example 1 analysis, we see no obvious pattern in the residual vs. predicted plot, suggesting the homogeneity of variances assumption is satisfied (Fig. 17.8). No outliers were present. The normal quantile plot suggests the normality assumption is satisfied.

Linear regression makes another key assumption, namely that the relationship between $Y$ and $X$ is linear. This assumption can be checked by examining a plot of $Y$ vs. $X$. What can be done if the relationship seems nonlinear? We can sometimes fix this problem by applying a transformation to $Y, X$, or both $Y$ and $X$, so that linear regression can be applied to the transformed data. This use of transformations greatly extends the utility of linear regression. Some commonly used transformations are $\log Y$ vs. $X, \log Y$ vs. $\log X, Y$ vs. $\log X$, and $1 / Y$ vs. $X$. A transformation that linearizes the data sometimes corrects for problems with the homogeneity of variances and normality assumptions.

A transformation may be selected based on prior information about the data and system. For example, a conservation biologist may be interested in the relationship between island area $A$ and the number of species $S$ on the island, and previous studies suggest that this relationship will be linear on a log scale (MacArthur \& Wilson 1967). Another approach is to try a number of transformations and chose the one that makes the data most linear. We will illustrate each approach with an example below.

In cases where no transformation can linearize the data, another possibility would be nonlinear regression (Juliano 1993). This type of analysis requires that the user specify a model $Y=f\left(X, \theta_{1}, \theta_{2}, \ldots\right)+\epsilon$ for the data, where $f$ is a function with parameters $\theta_{1}, \theta_{2}, \ldots$ to be estimated. SAS implements this type of nonlinear regression in proc nlin, while proc nlmixed allows for nonlinear functions as well as random effects and nonnormal distributions.

### 17.6.1 Species-area data - SAS demo

For many organisms there is a relationship between a defined area of habitat, such as an island, and the number of species found there. If $S$ is the number of species, and $A$ the area of habitat, then the model $S=c A^{z}$ seems to describe many data sets (MacArthur \& Wilson 1967). Applying the $\log _{10}$ function to both sides of this equation, we obtain

$$
\begin{equation*}
\log _{10} S=\log _{10} c+z \log _{10} A \tag{17.63}
\end{equation*}
$$

This form of the model is linear and suggests linear regression could be used to analyze species-area data. The SAS program listed below shows how these transformations can be applied to the bird fauna on archipelagos and islands of varying areas. The data are the number of species vs. island area (square miles) for 23 islands. The data were simulated to resemble Fig. 9 in MacArthur \& Wilson (1967). An extra observation is included with a missing value for the number of species, but an island area of 5000 square miles, to make proc glm calculate a confidence interval for the mean of this island.

We first conduct the analysis without any transformation, with the line $\mathrm{y}=$ species defining species as the dependent variable while $\mathrm{x}=$ area is the independent one. Examining the proc gplot graph, note the nonlinear nature of the relationship between the number of species and island area (Fig. 17.10). The picture improves after a $\log _{10}$ transformation is applied to both variables (Fig. 17.11).

Now that the linearity assumption is satisfied, we can interpret the rest of the SAS output (Fig. 17.13). We see that the number of species increased with island area $(\hat{\beta}=0.241)$ and the effect was highly significant $\left(F_{1,21}=\right.$ $148.16, P<0.0001)$. In terms of the original model, where $S=c A^{z}$, we see that $\hat{\beta}=0.241$ is also an estimate of $z$. The $R^{2}$ value is 0.876 , indicating that $87.6 \%$ of the variation is explained by the regression model. Confidence intervals are also provided for the intercept and slope.

The proc glm output also includes a predicted value $\hat{Y}_{i}=1.800$ at $X_{i}=$ 3.699, which corresponds to an island area of 5000 (see Fig. 17.14). We need to convert this predicted value to the original scale of measurement using antilogs. We have $\hat{S}_{i}=10^{\hat{Y}_{i}}=10^{1.800}=63.10$ species. So, we predict there would be 63 species on an island of 5000 square miles. The confidence interval for the mean is $(1.746,1.855)$, which we can similarly convert to $\left(10^{1.745}, 10^{1.855}\right)$ or $(55.72,71.61)$.

Examining the residual plots from this analysis, it appears the homogeneity of variances and normality assumptions were satisfied (Fig. 17.15).

```
                                    SAS Program
* SAprob2.sas;
title 'Linear regression for species-area data';
data sa;
    input species area;
    * Apply transformations here;
    y = log10(species);
    x = log10(area);
    datalines;
            28
        113480
        380358
        33252
        1010
            305
        37620
        4 7 6 2
            213
        2976
            2 3
            186
                4 2 3
        108512
            364
                269
        11163
            4 8 7
        445409
            7 0
        38309
        100873
        1354
        5 0 0 0
;
run;
* Print data set;
proc print data=sa;
run;
* Plot data and regression line;
proc gplot data=sa;
    plot y*x=1 y*x=2 y*x=3 / overlay vaxis=axis1 haxis=axis1;
    symbol1 i=none v=star c=black height=2 width=3;
```

```
    symbol2 i=rlclm v=none c=red height=2 width=3;
    symbol3 i=rlcli v=none c=blue height=2 width=3;
    axis1 label=(height=2) value=(height=2) width=3 major=(width=2) minor=none;
run;
* Regression analysis with confidence intervals;
proc glm plots=diagnostics data=sa;
    model y = x / clparm clm;
run;
* Regression analysis with prediction intervals;
proc glm data=sa;
    model y = x / clparm cli;
run;
quit;
```



Figure 17.10: SAprob2.sas - proc gplot


Figure 17.11: SAprob2.sas - proc gplot

## Linear regression for species-area data

| Obs | species | area | $\mathbf{y}$ | $\mathbf{x}$ |
| ---: | ---: | ---: | ---: | ---: |
| $\mathbf{1}$ | 15 | 28 | 1.17609 | 1.44716 |
| $\mathbf{2}$ | 104 | 113480 | 2.01703 | 5.05492 |
| $\mathbf{3}$ | 165 | 380358 | 2.21748 | 5.58019 |
| $\mathbf{4}$ | 116 | 33252 | 2.06446 | 4.52182 |
| $\mathbf{5}$ | 35 | 1010 | 1.54407 | 3.00432 |
| $\mathbf{6}$ | 33 | 305 | 1.51851 | 2.48430 |
| $\mathbf{7}$ | 78 | 37620 | 1.89209 | 4.57542 |
| $\mathbf{8}$ | 93 | 4762 | 1.96848 | 3.67779 |
| $\mathbf{9}$ | 50 | 213 | 1.69897 | 2.32838 |
| $\mathbf{1 0}$ | 76 | 2976 | 1.88081 | 3.47363 |
|  |  |  |  |  |

etc.
Figure 17.12: SAprob2.sas - proc print

## Linear regression for species-area data

## The GLM Procedure

| Number of Observations Read | 24 |
| :--- | :--- |
| Number of Observations Used | 23 |

## Linear regression for species-area data

The GLM Procedure
Dependent Variable: y

| Source | DF | Sum of Squares | Mean Square | F Value | Pr $>$ F |
| :--- | ---: | ---: | ---: | ---: | ---: |
| Model | 1 | 2.25182542 | 2.25182542 | 148.16 | $<.0001$ |
| Error | 21 | 0.31916133 | 0.01519816 |  |  |
| Corrected Total | 22 | 2.57098675 |  |  |  |


| R-Square | Coeff Var | Root MSE | y Mean |
| ---: | ---: | ---: | ---: |
| 0.875860 | 7.083042 | 0.123281 | 1.740507 |


| Source | DF | Type I SS | Mean Square | F Value | Pr > F |
| :--- | ---: | ---: | ---: | ---: | ---: |
| $\mathbf{x}$ | 1 | 2.25182542 | 2.25182542 | 148.16 | $<.0001$ |


| Source | DF | Type III SS | Mean Square | F Value | Pr > F |
| :--- | ---: | ---: | ---: | ---: | ---: |
| $\mathbf{x}$ | 1 | 2.25182542 | 2.25182542 | 148.16 | $<.0001$ |


| Parameter | Estimate | Standard <br> Error | t Value | $\operatorname{Pr}>\|\mathbf{t}\|$ | 95\% Confidence Limits |  |
| :--- | ---: | ---: | ---: | ---: | ---: | ---: |
| Intercept | 0.9102215097 | 0.07289411 | 12.49 | $<.0001$ | 0.7586299190 | 1.0618131004 |
| $\mathbf{x}$ | 0.2405722961 | 0.01976395 | 12.17 | $<.0001$ | 0.1994709127 | 0.2816736795 |

Figure 17.13: SAprob2.sas - proc glm

## Linear regression for species-area data

The GLM Procedure

| Observation | Observed | Predicted | Residual | 95\% Confidence Limits f | dicted Value |
| :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 1.17609126 | 1.25836764 | -0.08227638 | 1.16016869 | 1.35656659 |
| 2 | 2.01703334 | 2.12629506 | -0.10926172 | 2.04142998 | 2.21116013 |
| 3 | 2.21748394 | 2.25266125 | -0.03517730 | 2.15012264 | 2.35519985 |
| 4 | 2.06445799 | 1.99804559 | 0.06641240 | 1.92880841 | 2.06728278 |
| 5 | 1.54406804 | 1.63297800 | -0.08890996 | 1.57645124 | 1.68950477 |
| etc. |  |  |  |  |  |
| 20 | 1.27875360 | 1.35410098 | -0.07534738 | 1.26915398 | 1.43904798 |
| 21 | 2.04532298 | 2.01283671 | 0.03248627 | 1.94196673 | 2.08370669 |
| 22 | 2.18184359 | 2.11399114 | 0.06785245 | 2.03074815 | 2.19723412 |
| 23 | 1.74036269 | 1.66360220 | 0.07676049 | 1.60855303 | 1.71865138 |
| 24 |  | 1.80009122 |  | 1.74567238 | 1.85451005 |

Figure 17.14: SAprob2.sas - proc glm


Figure 17.15: SAprob2.sas - proc glm

### 17.6.2 Population growth rates - SAS demo

As another example of transformations, consider a study of the population growth of phytophagous mites on leaf sections. An experiment was conducted in which leaf sections are inoculated with a range of mite densities and the number of offspring recorded one generation later. The number of offspring per initial mite is the finite growth of the population, usually symbolized as $\lambda$. This is the dependent variable in the analysis while mite density is the independent one. The SAS program listed below gives the mite densities and the $\lambda$ values for this experiment.

We first conduct the analysis without any transformation. Looking at the plot of $Y(\lambda)$ vs. $X$ (density), we see a curvilinear relationship (Fig. 17.16). A transformation is clearly needed, but which one? A natural log transformation usually a good starting point for population data, both for growth rates and numbers. We begin by log-tranforming the dependent variable $\lambda$ and find that the plot is now linear (Fig. 17.17).

Interpreting the proc glm output below (Fig. 17.19), we see that $\lambda$ decreased with mite density $(\hat{\beta}=-0.020)$ and the effect was highly significant $\left(F_{1,15}=1695.22, P<0.0001\right)$. The $R^{2}$ value was 0.991 , indicating that almost all the variation in the data was explained by the regression line. It appears that the growth rate of the mites was adversely affected by their density, probably through competition for resources or other intraspecific interactions. The residual plots suggest the homogeneity of variances and normality assumptions were satisfied (Fig. 17.20).

```
                                    SAS Program
* logistic.sas;
title 'Linear regression for growth rate-density data';
data grd;
    input lambda density;
    * Apply transformations here;
    y = log(lambda);
    x = density;
    datalines;
    7.32 5
    4.82 15
    4 . 6 9 ~ 2 5
    3.90 35
    2.65 45
    2.52 55
    1.70 65
```

```
    1.68 75
    1.43 85
    1.07 95
    0.74105
    0.72115
    0.64125
    0.47 135
    0.40 145
    0.38155
    0.25 165
;
run;
* Print data set;
proc print data=grd;
run;
* Plot data and regression line;
proc gplot data=grd;
    plot y*x=1 y*x=2 y*x=3 / overlay vaxis=axis1 haxis=axis1;
    symbol1 i=none v=star c=black height=2 width=3;
    symbol2 i=rlclm v=none c=red height=2 width=3;
    symbol3 i=rlcli v=none c=blue height=2 width=3;
    axis1 label=(height=2) value=(height=2) width=3 major=(width=2) minor=none;
run;
* Regression analysis with confidence intervals;
proc glm plots=diagnostics data=grd;
    model y = x / clparm clm;
run;
* Regression analysis with prediction intervals;
proc glm data=grd;
    model y = x / clparm cli;
run;
quit;
```



Figure 17.16: logistic.sas - proc gplot


Figure 17.17: logistic.sas - proc gplot

## Linear regression for growth rate-density data

| Obs | lambda | density | $\mathbf{y}$ | $\mathbf{x}$ |
| ---: | ---: | ---: | ---: | ---: |
| $\mathbf{1}$ | 7.32 | 5 | 1.99061 | 5 |
| $\mathbf{2}$ | 4.82 | 15 | 1.57277 | 15 |
| $\mathbf{3}$ | 4.69 | 25 | 1.54543 | 25 |
| $\mathbf{4}$ | 3.90 | 35 | 1.36098 | 35 |
| $\mathbf{5}$ | 2.65 | 45 | 0.97456 | 45 |
| $\mathbf{6}$ | 2.52 | 55 | 0.92426 | 55 |
| $\mathbf{7}$ | 1.70 | 65 | 0.53063 | 65 |
| $\mathbf{8}$ | 1.68 | 75 | 0.51879 | 75 |
| $\mathbf{9}$ | 1.43 | 85 | 0.35767 | 85 |
| $\mathbf{1 0}$ | 1.07 | 95 | 0.06766 | 95 |
| $\mathbf{1 1}$ | 0.74 | 105 | -0.30111 | 105 |
| $\mathbf{1 2}$ | 0.72 | 115 | -0.32850 | 115 |
| $\mathbf{1 3}$ | 0.64 | 125 | -0.44629 | 125 |
| $\mathbf{1 4}$ | 0.47 | 135 | -0.75502 | 135 |
| $\mathbf{1 5}$ | 0.40 | 145 | -0.91629 | 145 |
| $\mathbf{1 6}$ | 0.38 | 155 | -0.96758 | 155 |
| $\mathbf{1 7}$ | 0.25 | 165 | -1.38629 | 165 |

Figure 17.18: logistic.sas - proc print

## Linear regression for growth rate-density data

The GLM Procedure

> | Number of Observations Read | 17 |
| :--- | :--- |
| Number of Observations Used | 17 |

## Linear regression for growth rate-density data

## The GLM Procedure

Dependent Variable: y

| Source | DF | Sum of Squares | Mean Square | F Value | Pr > F |
| :--- | ---: | ---: | ---: | ---: | ---: |
| Model | 1 | 16.36176928 | 16.36176928 | 1695.22 | $<.0001$ |
| Error | 15 | 0.14477544 | 0.00965170 |  |  |
| Corrected Total | 16 | 16.50654472 |  |  |  |


| R-Square | Coeff Var | Root MSE | y Mean |
| ---: | ---: | ---: | ---: |
| 0.991229 | 35.21791 | 0.098243 | 0.278958 |


| Source | DF | Type I SS | Mean Square | F Value | Pr > F |
| :--- | ---: | ---: | ---: | ---: | ---: |
| $\mathbf{x}$ | 1 | 16.36176928 | 16.36176928 | 1695.22 | $<.0001$ |


| Source | DF | Type III SS | Mean Square | F Value | Pr > F |
| :--- | ---: | ---: | ---: | ---: | ---: |
| $\mathbf{x}$ | 1 | 16.36176928 | 16.36176928 | 1695.22 | $<.0001$ |


| Parameter | Estimate | Standard <br> Error | $\boldsymbol{t}$ Value | $\operatorname{Pr}>\|\mathbf{t}\|$ | 95\% Confidence Limits |  |
| :--- | ---: | ---: | ---: | ---: | ---: | ---: |
| Intercept | 1.981131688 | 0.04771689 | 41.52 | $<.0001$ | 1.879425551 | 2.082837825 |
| $\mathbf{x}$ | -0.020025578 | 0.00048638 | -41.17 | $<.0001$ | -0.021062263 | -0.018988893 |

Figure 17.19: logistic.sas - proc glm


Figure 17.20: logistic.sas - proc glm

### 17.7 References

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SAS Institute Inc. (2016) SAS/GRAPH 9.4: Reference, Fifth Edition. SAS Institute Inc., Cary, NC.
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Searle, S. R. (1971) Linear Models. John Wiley \& Sons, Inc., New York, NY.

### 17.8 Problems

1. An experiment was conducted to measure the effect of density on the rate of egg laying in cowpea weevils. Ten different densities were used in the experiment, and the rate of egg laying determined for each density. The following data were obtained:

| Density | Eggs per day |
| ---: | ---: |
| 100 | 7.629 |
| 200 | 4.530 |
| 500 | 3.820 |
| 700 | 2.718 |
| 1200 | 2.403 |
| 1500 | 1.756 |
| 1700 | 1.772 |
| 2000 | 1.508 |
| 2200 | 1.518 |
| 2500 | 1.359 |

(a) Plot the rate of egg laying $(Y)$ vs. density $(X)$, and observe the nonlinear relationship between $Y$ and $X$. Find a transformation of $Y$ and/or $X$ that linearizes this relationship using SAS.
(b) For the transformed data, use SAS to plot a $95 \%$ confidence interval for the mean of $Y_{i}$ and a $95 \%$ prediction interval for a single value of $Y_{i}$. Label the intervals (confidence or prediction) on the gplot graph.
(c) Analyze the transformed data set using linear regression and SAS. In your SAS output, label the $95 \%$ confidence intervals for the intercept $(\alpha)$ and slope $(\beta)$ in your SAS printout.
(d) Interpret the results of the regression analysis. Is there a significant effect of density on the rate of egg production? What direction is the effect?
2. A zoologist wants to establish the relationship between the length of an animal and its weight. He wants to use length to predict weight in future studies, because length is easier to measure. The lengths and weights of a random sample of 20 animals were determined, yielding the following data:

| Length (mm) | Weight (g) |
| ---: | ---: |
| 14.7 | 1.65 |
| 19.9 | 4.86 |
| 15.8 | 2.04 |
| 19.0 | 3.53 |
| 8.4 | 0.32 |
| 10.2 | 0.46 |
| 13.5 | 1.68 |
| 22.1 | 6.24 |
| 16.2 | 1.85 |
| 8.2 | 0.28 |
| 10.1 | 0.48 |
| 19.8 | 4.18 |
| 20.6 | 4.77 |
| 22.0 | 6.10 |
| 18.1 | 2.78 |
| 22.4 | 5.26 |
| 10.5 | 0.55 |
| 14.5 | 1.56 |
| 11.9 | 1.07 |
| 14.7 | 1.74 |

(a) Plot the weight $(Y)$ vs. length $(X)$ using SAS, and observe the nonlinear relationship between $Y$ and $X$. Attach your graph of this relationship. Then, find a transformation of $Y$ and/or $X$ that linearizes this relationship. What transformation did you use? Attach your graph showing the transformed relationship.
(b) Analyze the transformed data using linear regression and SAS. Briefly interpret your results using $P$ values. Is there a significant effect of length on weight? What direction is the effect? Attach your program and output.
(c) For animals that are 21 mm long, find a $95 \%$ confidence interval for the mean weight.

