Topic 3

Correlation and Regression

In this section, we shall take a careful look at the nature of **linear relationships** found in the data used to construct a scatterplot. The first of these, **correlation**, examines this relationship in a symmetric manner. The second, **regression**, considers the relationship of a **response variable** as determined by one or more **explanatory variables**. Correlation focuses primarily of association, while regression is designed to help make predictions. Consequently, the first does not attempt to establish any cause and effect. The second is a often used as a tool to establish causality.

3.1 Covariance and Correlation

The **covariance** measures the linear relationship between a pair of quantitative measures

$$x_1, x_2, \ldots, x_n \quad \text{and} \quad y_1, y_2, \ldots, y_n$$

on the same sample of n individuals. Beginning with the definition of variance, the definition of covariance is similar to the relationship between the square of the norm $||v||^2$ of a vector v and the inner product $\langle v, w\rangle$ of two vectors v and w.

$$\text{cov}(x,y) = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y}).$$

vectors	**quantitative observations**
$\mathbf{v} = (v_1, \ldots, v_n)$ $\mathbf{w} = (w_1, \ldots, w_n)$	$\mathbf{x} = (x_1, \ldots, x_n)$ $\mathbf{y} = (y_1, \ldots, y_n)$
norm-squared $\|\|\mathbf{v}\|\|^2 = \sum_{i=1}^n v_i^2$	variance $s_x^2 = \frac{1}{n-1}\sum_{i=1}^n (x_i - \bar{x})^2$
norm $\|\|\mathbf{v}\|\|$	standard deviation s_x
inner product $\langle \mathbf{v}, \mathbf{w}\rangle = \sum_{i=1}^n v_i w_i$	covariance $\text{cov}(\mathbf{x}, \mathbf{y}) = \frac{1}{n-1}\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})$
cosine $\cos\theta = \frac{\langle \mathbf{v}, \mathbf{w}\rangle}{\|\|\mathbf{v}\|\| \, \|\|\mathbf{w}\|\|}$	correlation $r = \frac{\text{cov}(\mathbf{x}, \mathbf{y})}{s_x s_y}$

Table I: Analogies between vectors and quantitative observations.

A positive covariance means that the terms $(x_i - \bar{x})(y_i - \bar{y})$ in the sum are more likely to be positive than negative. This occurs whenever the x and y variables are more often both above or below the mean in tandem than not. Just like the situation in which the inner product of a vector with itself yields the square of the norm, the covariance of x with itself $\text{cov}(x,x) = s_x^2$ is the variance of x.

Exercise 3.1. *Explain in words what a negative covariance signifies, and what a covariance near 0 signifies.*

We next look at several exercises that call for algebraic manipulations of the formula for covariance or closely related functions.

Exercise 3.2. *Derive the alternative expression for the covariance:*

$$\text{cov}(x,y) = \frac{1}{n-1}\left(\sum_{i=1}^{n} x_i y_i - n\bar{x}\bar{y}\right).$$

Exercise 3.3. $\text{cov}(ax+b, cy+d) = ac \cdot \text{cov}(x, y)$. *How does a change in units (say from centimeters to meters) affect the covariance?*

Thus, covariance as a measure of association has the drawback that its value depends on the units of measurement. This shortcoming is remedied by using the correlation.

Definition 3.4. *The* **correlation**, r, *is the covariance of the standardized versions of x and y.*

$$r(x, y) = \frac{1}{n-1} \sum_{i=1}^{n} \left(\frac{x_i - \bar{x}}{s_x} \right) \left(\frac{y_i - \bar{y}}{s_y} \right) = \frac{\text{cov}(x, y)}{s_x s_y}.$$

The observations x and y are called **uncorrelated** *if $r(x, y) = 0$.*

Exercise 3.5. $r(ax + b, cy + d) = \pm r(x, y)$. *How does a change in units (say from centimeters to meters) affect the correlation? The plus sign occurs if $a \cdot c > 0$ and the minus sign occurs if $a \cdot c < 0$.*

Sometimes we will drop (x, y) if there is no ambiguity and simply write r for the correlation.

Exercise 3.6. *Show that*

$$s_{x+y}^2 = s_x^2 + s_y^2 + 2\text{cov}(x, y) = s_x^2 + s_y^2 + 2r s_x s_y. \tag{3.1}$$

Give the analogy between this formula and the law of cosines.

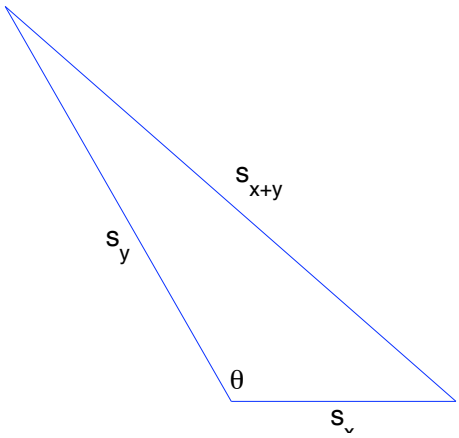


Figure 3.1: The analogy of the sample standard deviations and the law of cosines in equation (3.1). Here, the corrrelation $r = -\cos\theta$.

In particular if the two observations are uncorrelated we have the **Pythagorean identity**

$$s_{x+y}^2 = s_x^2 + s_y^2. \tag{3.2}$$

We will now look to uncover some of the properties of correlation. The next steps are to show that the correlation is always a number between -1 and 1 and to determine the relationship between the two variables in the case that the correlation takes on one of the two possible extreme values.

Exercise 3.7 (Cauchy-Schwarz inequality)**.** *For two sequences $v_1, \cdots, v_n$ and $w_1, \ldots, w_n$, show that*

$$\left(\sum_{i=1}^{n} v_i w_i \right)^2 \leq \left(\sum_{i=1}^{n} v_i^2 \right) \left(\sum_{i=1}^{n} w_i^2 \right). \tag{3.3}$$

Written in terms of norms and inner products, the Cauchy-Schwarz inequality becomes $\langle v, w \rangle^2 \leq ||v||^2 ||w||^2$.

(Hint: Consider the expression $\sum_{i=1}^{n} (v_i + w_i \zeta)^2 \geq 0$ as a quadratic expression in the variable ζ and consider the discriminant in the quadratic formula.) If the discriminant is zero, then we have equality in (3.3) and we have that $\sum_{i=1}^{n} (v_i + w_i \zeta)^2 = 0$ for exactly one value of ζ.

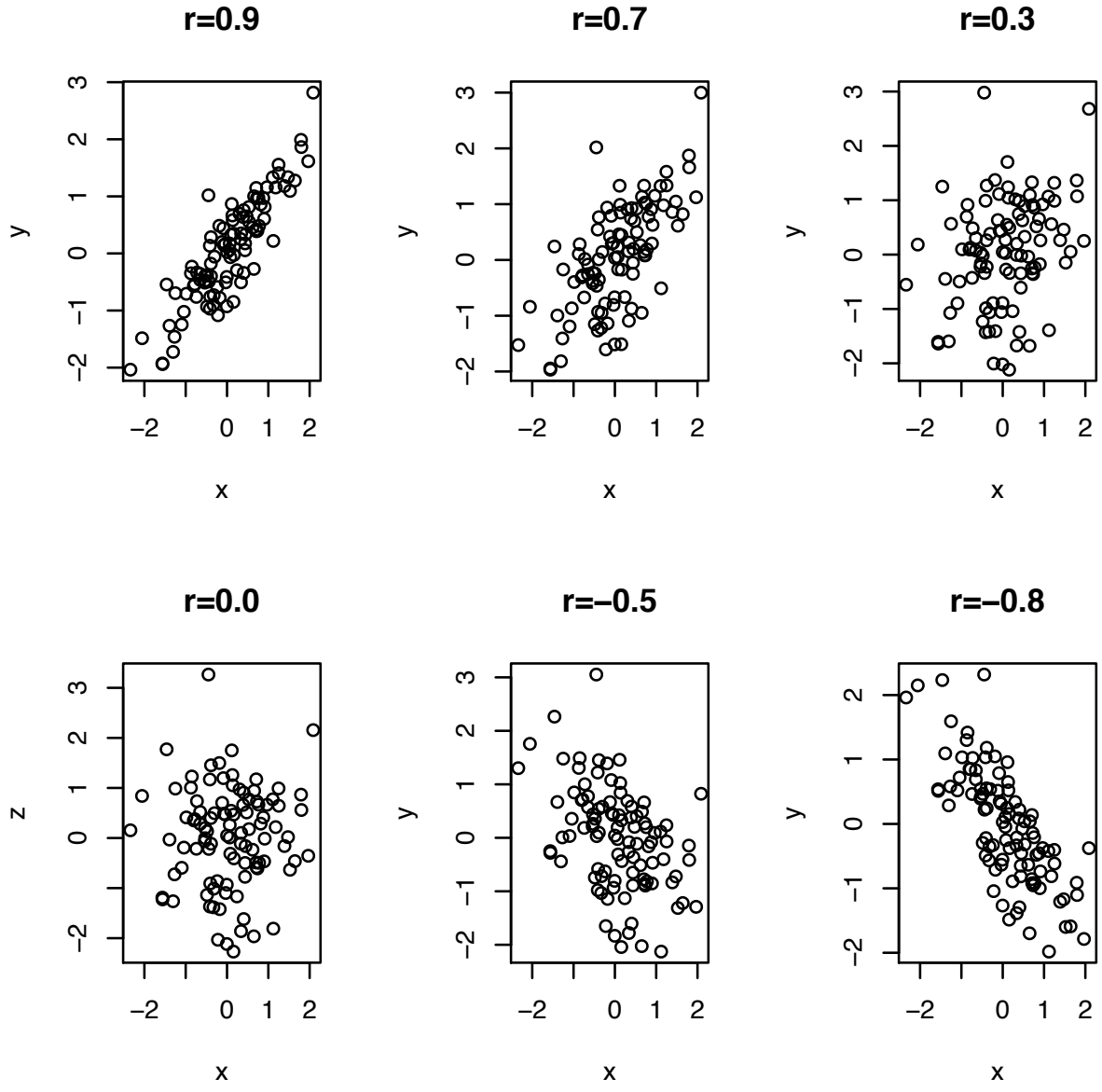
We shall use inequality (3.3) by choosing $v_i = x_i - \bar{x}$ and $w_i = y_i - \bar{y}$ to obtain

$$\left(\sum_{i=1}^{n} (x_i - \bar{x})(y_i - \bar{y}) \right)^2 \leq \left(\sum_{i=1}^{n} (x_i - \bar{x})^2 \right) \left(\sum_{i=1}^{n} (y_i - \bar{y})^2 \right),$$

$$\left(\frac{1}{n-1} \sum_{i=1}^{n} (x_i - \bar{x})(y_i - \bar{y}) \right)^2 \leq \left(\frac{1}{n-1} \sum_{i=1}^{n} (x_i - \bar{x})^2 \right) \left(\frac{1}{n-1} \sum_{i=1}^{n} (y_i - \bar{y})^2 \right),$$

$$\text{cov}(x, y)^2 \leq s_x^2 s_y^2$$

$$\frac{\text{cov}(x, y)^2}{s_x^2 s_y^2} \leq 1$$



[t!]

Figure 3.2: Scatterplots showing differing levels of the correlation r

Consequently, we find that

$$r^2 \le 1 \quad \text{or} \quad -1 \le r \le 1.$$

When we have $|r| = 1$, then we have equality in (3.3). In addition, for some value of ζ we have that

$$\sum_{i=1}^{n}((x_i - \bar{x}) + (y_i - \bar{y})\zeta)^2 = 0.$$

The only way for a sum of nonnegative terms to add to give zero is for each term in the sum to be zero, i.e.,

$$(x_i - \bar{x}) + (y_i - \bar{y})\zeta = 0, \quad \text{for all } i = 1, \dots, n. \tag{3.4}$$

Thus x_i and y_i are linearly related.

$$y_i = \alpha + \beta x_i.$$

In this case, the sign of r is the same as the sign of β.

Exercise 3.8. *For an alternative derivation that $-1 \le r \le 1$. Use equation (3.1) with x and y standardized observations. Use this to determine ζ in equation (3.4) (*Hint: *Consider the separate cases s^2_{x+y} for the $r = -1$ and s^2_{x-y} for the $r = 1$.)*

We can see how this looks for simulated data. Choose a value for `r` between -1 and $+1$.

```
>x<-rnorm(100)
>z<-rnorm(100)
>y<-r*x + sqrt(1-r^2)*z
```

Example of plots of the output of this simulation are given in Figure 3.1. For the moment, the object of this simulation is to obtain an intuitive feeling for differing values for correlation. We shall soon see that this is the simulation of pairs of normal random variables with the desired correlation. From the discussion above, we can see that the scatterplot would lie on a straight line for the values $r = \pm 1$.

For the *Archeopteryx* data on bone lengths, we have the correlation

```
> cor(femur, humerus)
[1] 0.9941486
```

Thus, the data land very nearly on a line with positive slope.

For the banks in 1974, we have the correlation

```
> cor(income,assets)
[1] 0.9325191
```

3.2 Linear Regression

Covariance and correlation are measures of linear association. For the *Archeopteryx* measurements, we learn that the relationship in the length of the femur and the humerus is very nearly linear.

We now turn to situations in which the value of the first variable x_i will be considered to be **explanatory** or **predictive**. The corresponding observation y_i, taken from the input x_i, is called the **response**. For example, can we **explain** or **predict** the income of banks from its assets? In this case, *assets* is the explanatory variable and income is the response.

In **linear regression**, the response variable is linearly related to the explanatory variable, but is subject to deviation or to error. We write

$$y_i = \alpha + \beta x_i + \epsilon_i. \tag{3.5}$$

Our goal is, given the data, the x_i's and y_i's, to find α and β that determines the line having the best fit to the data. The principle of **least squares regression** states that the best choice of this linear relationship is the one that

minimizes the square in the *vertical distance* from the y values in the data and the y values on the regression line. This choice reflects the fact that the values of x are set by the experimenter and are thus assumed known. Thus, the "error" appears in the value of the response variable y.

This principle leads to a minimization problem for

$$SS(\alpha, \beta) = \sum_{i=1}^{n} \epsilon_i^2 = \sum_{i=1}^{n} (y_i - (\alpha + \beta x_i))^2. \tag{3.6}$$

In other words, given the data, determine the values for α and β that minimizes the **sum of squares** SS. Let's the denote by $\hat{\alpha}$ and $\hat{\beta}$ the value for α and β that minimize SS.

Take the partial derivative with respect to α.

$$\frac{\partial}{\partial \alpha} SS(\alpha, \beta) = -2 \sum_{i=1}^{n} (y_i - \alpha - \beta x_i)$$

At the values $\hat{\alpha}$ and $\hat{\beta}$, this partial derivative is 0. Consequently

$$0 = \sum_{i=1}^{n} (y_i - \hat{\alpha} - \hat{\beta} x_i) \quad \sum_{i=1}^{n} y_i = \sum_{i=1}^{n} (\hat{\alpha} - \hat{\beta} x_i).$$

Now, divide by n.

$$\bar{y} = \hat{\alpha} + \hat{\beta} \bar{x}. \tag{3.7}$$

Thus, we see that the **center of mass point** $(\bar{x}, \bar{y})$ is on the regression line. To emphasize this fact, we rewrite (3.5) in **slope-point** form.

$$y_i - \bar{y} = \beta (x_i - \bar{x}) + \epsilon_i. \tag{3.8}$$

We then apply this to the sums of squares criterion (3.6) to obtain a condition that depends on β,

$$\tilde{SS}(\beta) = \sum_{i=1}^{n} \epsilon_i^2 = \sum_{i=1}^{n} ((y_i - \bar{y}) - \beta (x_i - \bar{x}))^2. \tag{3.9}$$

Now, differentiate with respect to β and set this equation to zero for the value $\hat{\beta}$.

$$\frac{d}{d\beta} \tilde{SS}(\beta) = -2 \sum_{i=1}^{n} ((y_i - \bar{y}) - \hat{\beta} (x_i - \bar{x}))(x_i - \bar{x}) = 0.$$

Thus,

$$\sum_{i=1}^{n} (y_i - \bar{y})(x_i - \bar{x}) = \hat{\beta} \sum_{i=1}^{n} (x_i - \bar{x})^2$$

$$\frac{1}{n-1} \sum_{i=1}^{n} (y_i - \bar{y})(x_i - \bar{x}) = \hat{\beta} \frac{1}{n-1} \sum_{i=1}^{n} (x_i - \bar{x})^2$$

$$\text{cov}(x, y) = \hat{\beta} \text{var}(x)$$

Now solve for $\hat{\beta}$.

$$\hat{\beta} = \frac{\text{cov}(x, y)}{\text{var}(x)}. \tag{3.10}$$

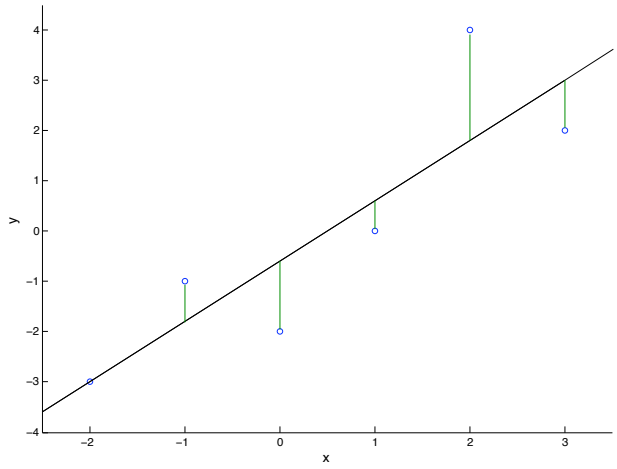


Figure 3.3: Scatterplot and the regression line for the six point data set below. The regression line is the choice that minimizes the square of the vertical distances from the observation values to the line, indicated here in green. Notice that the total length of the positive residuals (the lengths of the green line segments above the regression line) is equal to the total length of the negative residuals. This property is derived in equation (3.11).

In summary, to determine the **regression line**.

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

we use (3.10) to determine $\hat{\beta}$ and then (3.7) to solve for

$$\hat{\alpha} - \hat{\beta}\bar{x} - \bar{y}.$$

We call $\hat{y}_i$ the **fit** for the value x_i.

Example 3.9. *Let's begin with 6 points and derive by hand the equation for regression line.*

x	-2	-1	0	1	2	3
y	-3	-1	-2	0	4	2

Add the x and y values and divide by $n = 6$ to see that $\bar{x} = 0.5$ and $\bar{y} = 0$.

x_i	y_i	$x_i - \bar{x}$	$y_i - \bar{y}$	$(x_i - \bar{x})(y_i - \hat{y})$	$(x_i - \bar{x})^2$
-2	-3	-2.5	-3	7.5	6.25
-1	-1	-1.5	-1	1.5	2.25
0	-2	-0.5	-2	1.0	0.25
1	0	0.5	0	0.0	0.25
2	4	1.5	4	6.0	2.25
3	2	2.5	2	5.0	6.25
sum		0	0	$\text{cov}(x, y) = 21/5$	$\text{var}(x) = 17.50/5$

Thus,

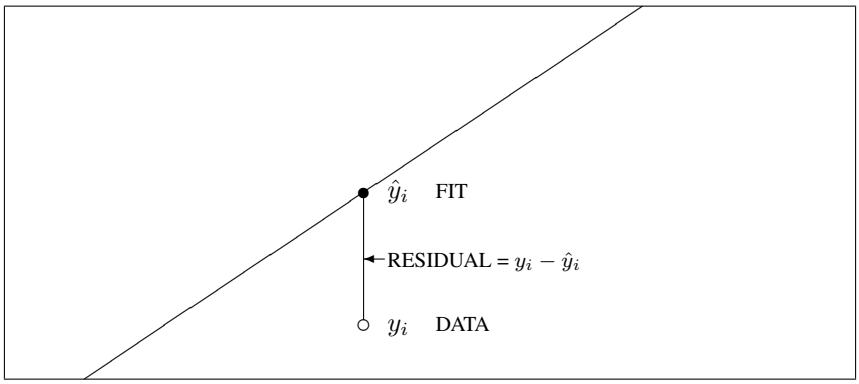
$$\hat{\beta} = \frac{21/5}{17.5/5} = 1.2 \quad \textit{and} \quad 0 = \hat{\alpha} + 1.2 \times 0.5 = \hat{\alpha} + 0.6 \quad \textit{or} \quad \hat{\alpha} = -0.6$$

As seen in this example, fits, however rarely perfect. The difference between the fit and the data is an estimate $\hat{\epsilon}_i$ for the error ϵ_i. This difference is called the **residual**. So,

$$\text{RESIDUAL}_i = \text{DATA}_i - \text{FIT}_i = y_i - \hat{y}_i$$

or, by rearranging terms,

$$\text{DATA}_i = \text{FIT}_i + \text{RESIDUAL}_i, \quad \textit{or} \quad y_i = \hat{y}_i + \hat{\epsilon}_i.$$



We can rewrite equation (3.6) with $\hat{\epsilon}_i$ estimating the error in (3.5).

$$0 = \sum_{i=1}^{n}(y_i - \hat{\alpha} - \hat{\beta}x_i) = \sum_{i=1}^{n}(y_i - \hat{y}_i) = \sum_{i=1}^{n}\hat{\epsilon}_i \tag{3.11}$$

to see that the sum of the residuals is 0. Thus, we started with a criterion for a line of best fit, namely, least squares, and discover that a consequence of this criterion the regression line has the property that the sum of the residual values is 0. This is illustrated in Figure 3.3.

Let's check this property for the example above.

	DATA	FIT	RESIDUAL
x_i	y_i	$\hat{y}_i$	$\hat{y}_i - y_i$
-2	-3	-3.0	0
-1	-1	-1.8	0.8
0	-2	-0.6	-1.4
1	0	0.6	-0.6
2	4	1.8	2.2
3	2	3.0	-1.0
	total		0

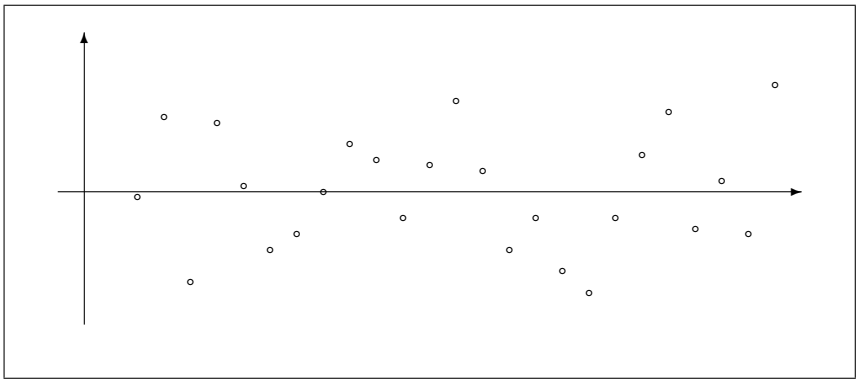
Generally speaking, we will look at a **residual plot**, the plot of the residuals versus the explanatory variable, to assess the appropriateness of a regression line. Specifically, we will look for circumstances in which the explanatory variable and the residuals have no systematic pattern.

Exercise 3.10. *Use* R *to perform the following operations on the data set in Example 3.9.*

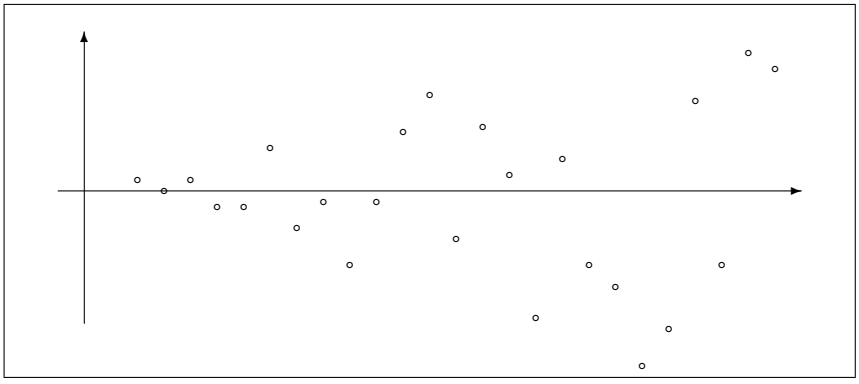
1. *Enter the data and make a scatterplot.*
2. *Use the* `lm` *command to find the equation of the regression line.*
3. *Use the* `abline` *command to draw the regression line on the scatterplot.*
4. *Use the* `resid` *and the* `predict` *command command to find the residuals and place them in a* `data.frame` *with* `x` *and* `y`

5. *Draw the residual plot and use* `abline` *to add the horizontal line at 0.*

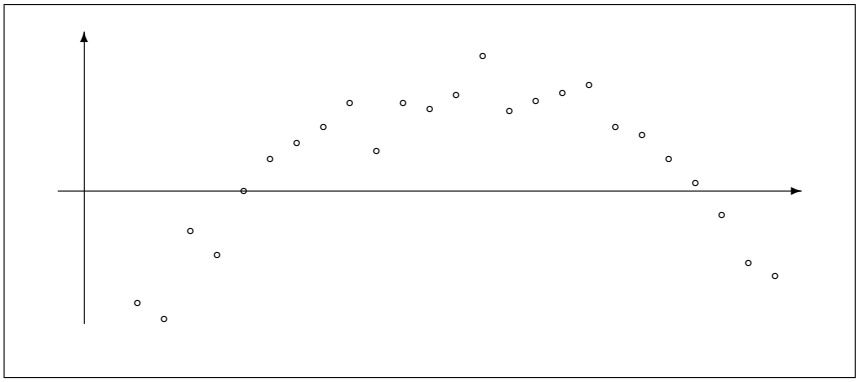
We next show three examples of the residuals plotting against the value of the explanatory variable.



Regression fits the data well - homoscedasticity



Prediction is less accurate for large x, an example of heteroscedasticity



Data has a curve. A straight line fits the data poorly.

For any value of x, we can use the regression line to estimate or **predict** a value for y. We must be careful in using this prediction outside the range of x. This **extrapolation** will not be valid if the relationship between x and y is not known to be linear in this extended region.

Example 3.11. *For the 1974 bank data set, the regression line*

$$\widehat{income} = 7.680 + 4.975 \cdot assets.$$

So, each dollar in assets brings in about $5 income.

For a bank having 10 billion dollars in assets, the predicted income is 56.430 billion dollars. However, if we extrapolate this down to very small banks, we would predict nonsensically that a bank with no *assets would have an income of 7.68 billion dollars. This illustrates the caution necessary to perform a reliable prediction through an extrapolation.*

In addition for this data set, we see that three banks have assets much greater than the others. Thus, we should consider examining the regression lines omitting the information from these three banks. If a small number of observations has a large impact on our results, we call these points **influential**.

Obtaining the regression line in R *is straightforward:*

```
> lm(income~assets)

Call:
lm(formula = income ~ assets)

Coefficients:
(Intercept)       assets
      7.680        4.975
```

Example 3.12 (regression line in standardized coordinates)**.** *Sir Francis Galton was the first to use the term* **regression** *in his study* Regression towards mediocrity in hereditary stature*. The rationale for this term and the relationship between regression and correlation can be best seen if we convert the observations into a standardized form.*

First, write the regression line to point-slope form.

$$\hat{y}_i - \bar{y} = \hat{\beta}(x_i - \bar{x}).$$

Because the slope

$$\hat{\beta} = \frac{\text{cov}(x,y)}{\text{var}(x)} = \frac{r s_x s_y}{s_x^2} = \frac{r s_y}{s_x},$$

we can rewrite the point-slope form as

$$\hat{y}_i - \bar{y} = \frac{r s_y}{s_x}(x_i - \bar{x}) \quad \textit{or} \quad \frac{\hat{y}_i - \bar{y}}{s_y} = r\frac{x_i - \bar{x}}{s_x}, \quad \hat{y}_i^* = r x_i^*. \tag{3.12}$$

where the asterisk is used to indicate that we are stating our observations in standardized form. In words, if we use this standardized form, then the slope of the regression line is the correlation.

For Galton's example, let's use the height of a male as the explanatory variable and the height of his adult son as the response. If we observe a correlation $r = 0.6$ and consider a man whose height is 1 standard deviation above the mean, then we predict *that the son's height is 0.6 standard deviations above the mean. If a man whose height is 0.5 standard deviation below the mean, then we* predict *that the son's height is 0.3 standard deviations below the mean. In either case, our prediction for the son is a height that is closer to the mean then the father's height. This is the "regression" that Galton had in mind.*

From the discussion above, we can see that if we reverse the role of the explanatory and response variable, then we change the regression line. This should be intuitively obvious since in the first case, we are minimizing the total square vertical distance and in the second, we are minimizing the total square horizontal distance. In the most extreme circumstance, $\text{cov}(x,y) = 0$. In this case, the value x_i of an observation is no help in predicting the response variable.

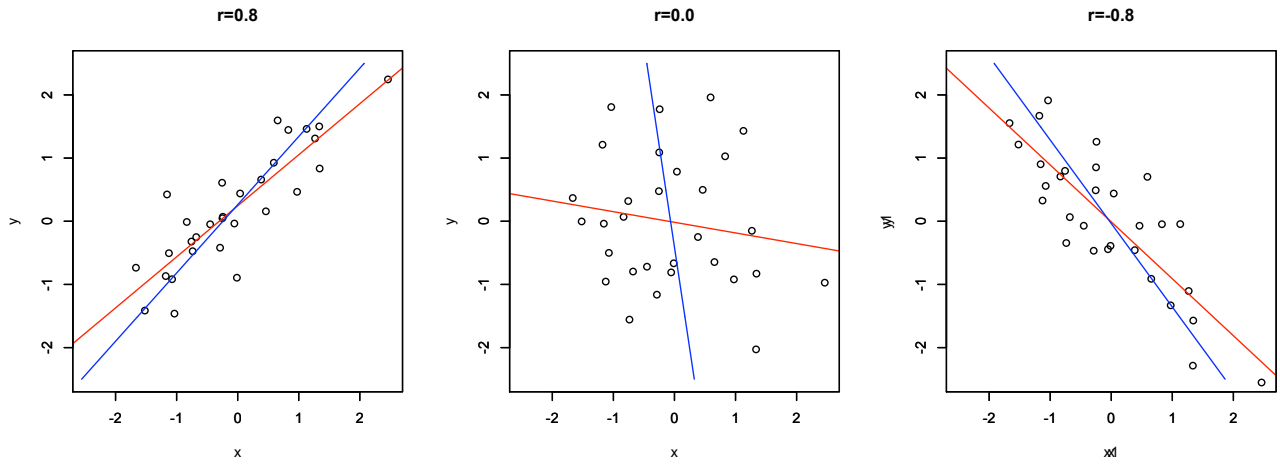


Figure 3.4: Scatterplots of standardized variables and their regression lines. The red lines show the case in which x is the explanatory variable and the blue lines show the case in which y is the explanatory variable.

Thus, as the formula states, when x is the explanatory variable the regression line has slope 0 - it is a horizontal line through $\bar{y}$. Correspondingly, when y is the explanatory variable, the regression is a vertical line through $\bar{x}$. Intuitively, if x and y are uncorrelated, then the best prediction we can make for y_i given the value of x_i is just the sample mean $\bar{y}$ and the best prediction we can make for x_i given the value of y_i is the sample mean $\bar{x}$.

More formally, the two regression equations are

$$\hat{y}_i^* = rx_i^* \quad \text{and} \quad \hat{x}_i^* = ry_i^*.$$

These equations have slopes r and $1/r$. This is shown by example in Figure 3.2.

Exercise 3.13. *Compute the regression line for the 6 pairs of observations above assuming that y is the explanatory variable. Show that the two region lines differ by showing that the product of the slopes in not equal to one.*

Exercise 3.14. *Continuing the previous example, let $\hat{\beta}_x$ be the slope of the regression line obtained from regressing y on x and $\hat{\beta}_y$ be the slope of the regression line obtained from regressing x on y. Show that the product of the slopes $\hat{\beta}_x\hat{\beta}_y = r^2$, the square of the correlation.*

Because the point $(\bar{x}, \bar{y})$ is on the regression line, we see from the exercise above that two regression lines coincide precisely when the slopes are reciprocals, namely precisely when $r^2 = 1$. This occurs for the values $r = 1$ and $r = -1$.

Exercise 3.15. *Show that the FIT, $\hat{y}$, and the RESIDUALS, $y - \hat{y}$ are uncorrelated.*

Let's again write the regression line in point slope form

$$\text{FIT}_i - \bar{y} = \hat{y}_i - \bar{y} = r\frac{s_y}{s_x}(x_i - \bar{x}).$$

Using the quadratic identity for variance we find that

$$s_{FIT}^2 = r^2\frac{s_y^2}{s_x^2}s_x^2 = r^2 s_y^2 = r^2 s_{DATA}^2.$$

Thus, the variation in the FIT is reduced from the variation in the DATA by a factor of r^2 and

$$r^2 = \frac{s_{FIT}^2}{s_{DATA}^2}.$$

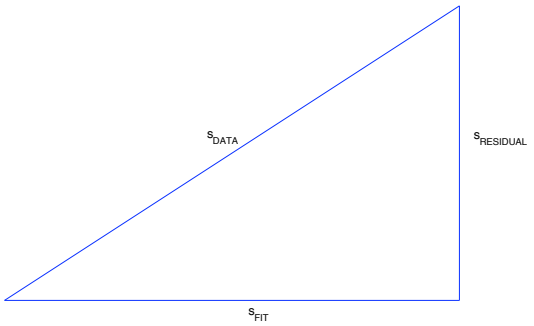


Figure 3.5: The relationship of the standard deviations of the DATA, the FIT, and the RESIDUALS. $s_{DATA}^2 = s_{FIT}^2 + s_{RESID}^2 = r^2 s_{DATA}^2 + (1 - r^2)s_{DATA}^2$. In this case, we say that r^2 of the variation in the response variable is due to the fit and the rest $1 - r^2$ is due to the residuals.

Exercise 3.16. *Use the equation above to show that*

$$r^2 = \frac{\sum_{i=1}^{n}(\hat{y}_i - \bar{y})^2}{\sum_{i=1}^{n}(y_i - \bar{y})^2}.$$

When the straight line fits the data well, the FIT and the RESIDUAL are uncorrelated and the magnitude of the residual does not depend on the value of the explanatory variable. We have, in this circumstance, from equation (3.2), the Pythagorean identity, that

$$s^2_{DATA} = s^2_{FIT} + s^2_{RESID} = r^2 s^2_{DATA} + s^2_{RESIDUAL}$$

$$s^2_{RESIDUAL} = (1 - r^2)s^2_{DATA}.$$

Thus, r^2 of the variance in the data can be explained by the fit. As a consequence of this computation, many statistical software tools report r^2 as a part of the linear regression analysis. In the case the remaining $1 - r^2$ of the variance in the data is found in the residuals.

Exercise 3.17. *For some situations, the circumstances dictate that the line contain the origin ($\alpha = 0$). Use a least squares criterion to show that the slope of the regression line*

$$\hat{\beta} = \frac{\sum_{i=1}^{n} x_i y_i}{\sum_{i=1}^{n} x_i^2}.$$

R accommodates this circumstance with the commands `lm(y~x-1)` or `lm(y~0+x)`. Note that in this case, the sum of the residuals is not necessarily equal to zero. For least squares regression, this property followed from $\partial SS(\alpha, \beta)/\partial\alpha = 0$ where α is the y-intercept.

3.2.1 Transformed Variables

For pairs of observations $(x_1, y_1), \ldots, (x_n, y_n)$, the linear relationship may exist not with these variables, but rather with transformation of the variables. In this case we have,

$$\psi(y_i) = \alpha + \beta g(x_i) + \epsilon_i. \tag{3.13}$$

We then perform linear regression on the variables $\tilde{y} = \psi(y)$ and $\tilde{x} = g(x)$ using the least squares criterion. If

$$y_i = Ae^{kx_i + \epsilon_i},$$

we take logarithms,

$$\ln y_i = \ln A + kx_i + \epsilon_i$$

So, in (3.13), $\psi(y_i) = \ln y_i$, $g(x_i) = x_i$ is the transformation of the data, The parameters are $\alpha = \ln A$ and $\beta = k$.

Before we look at an example, let's review a few basic properties of **logarithms**

Remark 3.18 (logarithms)**.** *We will use both* log*, the base 10* **common logarthm***, and* ln*, the base* e **natural logarithm***. Common logarithms help us see orders of magnitude. For example, if* $\log y = 5$*, then we know that* $y = 10^5 = 100,000$*. if* $\log y = -1$*, then we know that* $y = 10^{-1} = 1/10$*. We will use natural logarithms to show instantaneous rates of growth. Consider the differential equation*

$$\frac{dy}{dt} = ky.$$

We are saying that the instantaneous rate of growth of y *is proportional to* y *with constant of proportionality* k*. The solution to this equation is*

$$y = y_0 e^{kt} \qquad \textit{or} \qquad \ln y = \ln y_0 + kt$$

where y_0 is the initial value for y. This gives a linear relationship between $\ln y$ and t. The two values of logarithm have a simple relationship. If we write

$$x = 10^a. \text{ Then } \log x = a \text{ and } \ln x = a \ln 10.$$

Thus, by substituting for a, we find that

$$\ln x = \log x \cdot \ln 10 = 2.3026 \log x.$$

In R*, the command for the natural logarithm of* `x` *is* `log(x)`*. For the common logarithm, it is* `log(x,10)`*.*

Example 3.19. *In the data on world oil production, the relationship between the explanatory variable and response variable is nonlinear but can be made to be linear with a simple transformation, the common logarithm. Call the new response variable* logbarrel*. The explanatory variable remains* year*. With these variables, we can use a regression line to help describe the data. Here the model is*

$$\log y_i = \alpha + \beta x_i + \epsilon_i. \tag{3.14}$$

Regression is the first example of a class of statistical models called **linear models***. At this point we emphasize that* **linear** *refers to the appearance of the parameters α and β linearly in the function (3.14). This acknowledges that, in this circumstance, the values x_i and y_i are known. Indeed, they are the data. Our goal is to give an estimate $\hat{\alpha}$ and $\hat{\beta}$ for the values of α and β.*

Thus, R *uses the command* `lm`*. Here is the output.*

```
> summary(lm(logbarrel~year))

Call:
lm(formula = logbarrel ~ year)

Residuals:
     Min       1Q   Median       3Q      Max
-0.25562 -0.03390  0.03149  0.07220  0.12922

Coefficients:
              Estimate Std. Error t value Pr(>|t|)
(Intercept) -5.159e+01  1.301e+00  -39.64   <2e-16 ***
year         2.675e-02  6.678e-04   40.05   <2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.1115 on 27 degrees of freedom
Multiple R-Squared: 0.9834,Adjusted R-squared: 0.9828
F-statistic:  1604 on 1 and 27 DF,  p-value: < 2.2e-16
```

Note that the output states $r^2 = 0.9828$. Thus, the correlation is $r = 0.9914$ is very nearly one and so the data lies very close to the regression line.

For world oil production, we obtained the relationship

$$\widehat{\log(barrel)} = -51.59 + 0.02675 \cdot year.$$

If we rewrite the equation in exponential form, we obtain

$$\widehat{barrel} = A10^{0.02675 \cdot year} = Ae^{\hat{k} \cdot year}.$$

Thus, $\hat{k}$ gives the instantaneous growth rate that best fits the data. This is obtained by converting from a common logarithm to a natural logarithm.

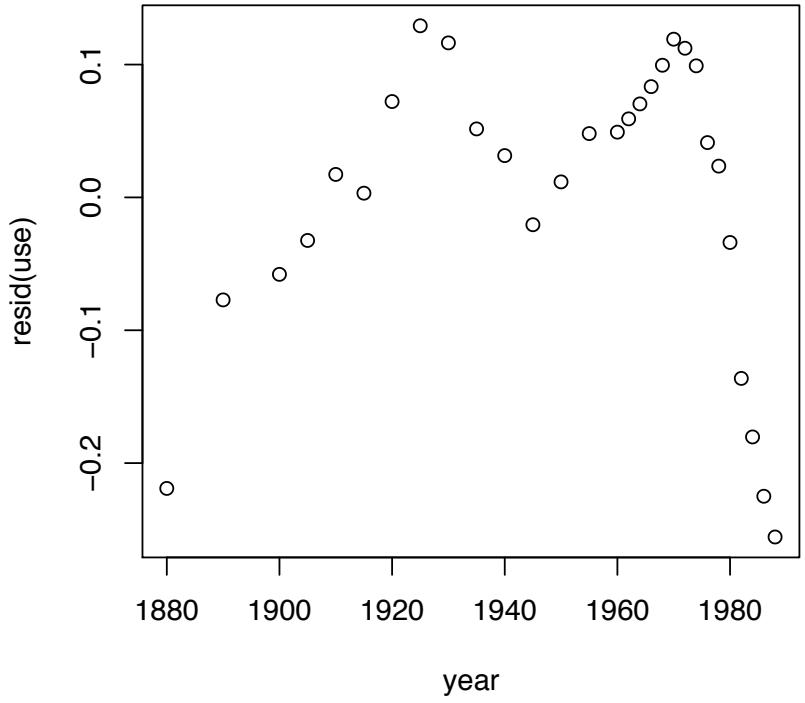
$$\hat{k} = 0.02675 \ln 10 = 0.0616$$

.

Consequently, the use of oil sustained a growth of 6% per year over a span of a hundred years.

Next, we will look for finer scale structure by examining the residual plot.

```
> use<-lm(logbarrel~year)
> plot(year,resid(use))
```



Exercise 3.20. *Remove the data points after the oil crisis of the mid 1970s, find the regression line and the instantaneous growth rate that best fits the data. Look at the residual plot and use fact about American history to explain why the residuals increase until 1920's, decrease until the early 1940's and increase again until the early 1970's.*

Example 3.21 (Michaelis-Menten Kinetics)**.** *In this example, we will have to use a more sophisticated line of reasoning to create a linear relationship between a explanatory and response variable. Consider the chemical reaction in which an enzyme catalyzes the action on a substrate.*

$$E + S \underset{k_{-1}}{\overset{k_1}{\rightleftarrows}} ES \xrightarrow{k_2} E + P \tag{3.15}$$

Here

- E_0 *is the total amount of enzyme.*
- E *is the free enzyme.*
- S *is the substrate.*
- ES *is the substrate-bound enzyme.*
- P *is the product.*
- $V = d[P]/dt$ *is the production rate.*

The numbers above or below the arrows gives the reaction rates. Using the symbol $[\,\cdot\,]$ *to indicate* **concentration***, notice that the enzyme,* E_0*, is either free or bound to the substrate. Its total concentration is, therefore,*

$$[E_0] = [E] + [ES], \quad \textit{and, thus} \quad [E] = [E_0] - [ES] \tag{3.16}$$

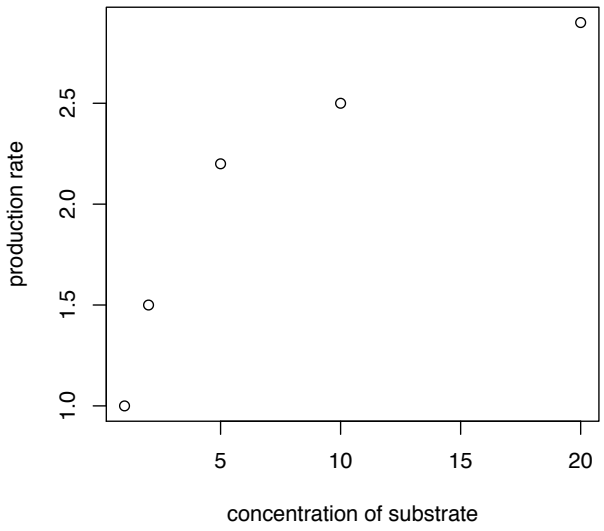
Our goal is to relate the production rate V *to the substrate concentration* $[S]$*.*

The **law of mass action** *turns the chemical reactions in (3.15) into differential equations. In particular, the reactions, focusing on the substrate-bound enzyme and the product, gives the equations*

$$\frac{d[ES]}{dt} = k_1[E][S] - [ES](k_{-1} + k_2) \quad \textit{and} \quad V = \frac{d[P]}{dt} = k_2[ES] \tag{3.17}$$

We can meet our goal if we can find an equation for $V = k_2[ES]$ *that depends only on* $[S]$*, the substrate concentration. Let's look at data,*

$[S]$ (mM)	1	2	5	10	20
V (nmol/sec)	1.0	1.5	2.2	2.5	2.9



If we wish to use linear regression, then we will have to transform the data. In this case, we will develop the Michaelis-Menten transformation applied to situations in which the concentration of the substrate-bound enzyme (and hence also the unbound enzyme) changes much more slowly than those of the product and substrate.

$$0 \approx \frac{d[ES]}{dt}$$

In words, the substrate-bound enzyme is nearly in steady state. Using the law of mass action equation (3.17) for $d[ES]/dt$*, we can rearrange terms to conclude that*

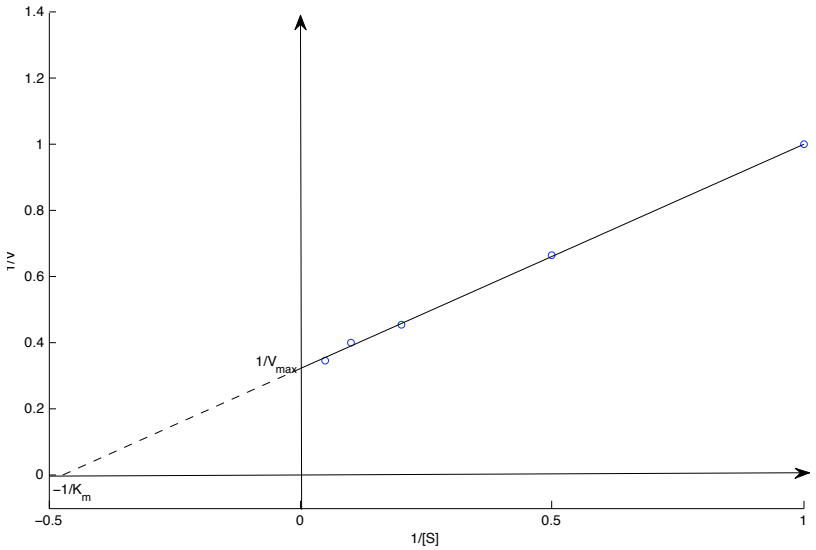


Figure 3.6: Lineweaver-Burke double reciprocal plot for the data presented above. The y-intercept gives the reciprocal of the maximum production. The dotted line indicates that negative concentrations are not physical. Nevertheless, the x-intercept give the negative reciprocal of the Michaelis constant.

$$[ES] \approx \frac{k_1[E][S]}{k_{-1}+k_2} = \frac{[E][S]}{K_m}. \tag{3.18}$$

The ratio $K_m = (k_{-1}+k_2)/k_1$ of the rate of loss of the substrate-bound enzyme to its production is called the **Michaelis constant**. *We have now met our goal part way, V is a function of $[S]$, but it is also stated as a function of $[E]$.*

Thus, we have $[E]$ as a function of $[ES]$. Now, if we combine this with (3.18) and (3.16) and solve for $[ES]$, then

$$[ES] \approx \frac{([E_0]-[ES])[S]}{K_m}, \quad [ES] \approx [E_0]\frac{[S]}{K_m+[S]}$$

Under this approximation, the production rate of the product is:

$$V = \frac{d[P]}{dt} = k_2[ES] = k_2[E_0]\frac{[S]}{K_m+[S]} = V_{\max}\frac{[S]}{K_m+[S]}$$

Here, $V_{\max} = k_2[E_0]$ is the maximum production rate. (To see this, let the substrate concentration $[S] \to \infty$.) To perform linear regression, we need to have a function of V be linearly related to a function of $[S]$. This is achieved via taking the reciprocal of both sides of this equation.

$$\frac{1}{V} = \frac{K_m+[S]}{V_{\max}[S]} = \frac{1}{V_{\max}} + \frac{K_m}{V_{\max}}\frac{1}{[S]} \tag{3.19}$$

Thus, we have a linear relationship between

$$\frac{1}{V}, \text{the response variable, and } \frac{1}{[S]}, \text{the explanatory variable}$$

subject to experimental error. The **Lineweaver-Burke double reciprocal plot** *provides a useful method for analysis of the Michaelis-Menten equation. See Figure 3.6.*

For the data,

$[S]$ (mM)	1	2	5	10	20
V (nmol/sec)	1.0	1.5	2.2	2.5	2.9

The regression line is

$$\frac{1}{V} = 0.3211 + \frac{1}{[S]}0.6813.$$

Here are the R *commands*

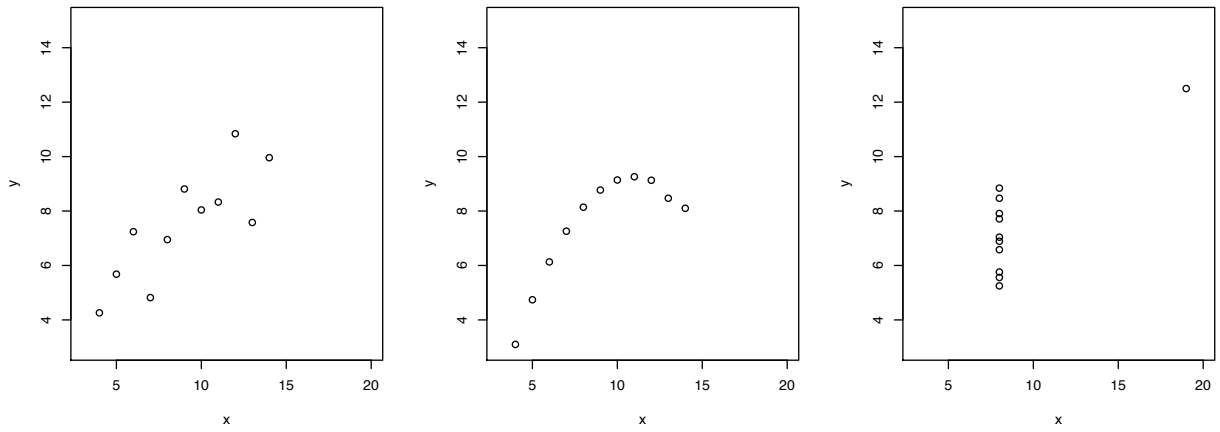
```
> S<-c(1,2,5,10,20)
> V<-c(1.0,1.5,2.2,2.5,2.9)
> Sinv<-1/S
> Vinv<-1/V
> lm(Vinv~Sinv)

Call:
lm(formula = Vinv ~ Sinv)

Coefficients:
(Intercept)         Sinv
     0.3211       0.6813
```

Using (3.19), we find that $V_{\max} = 3.1141$ *and* $K_m = 0.4713$. *With more access to computational software, this method is not used as much as before. The measurements for small values of the concentration (and thus large value of* $1/[S]$*) are more variable and consequently the residuals are likely to be heteroscedastic. We look in the next section for an alternative approach, namely nonlinear regression.*

Example 3.22 (Frank Amscombe)**.** *Consider the three data sets:*

x	10	8	13	9	11	14	6	4	12	7	5
y	8.04	6.95	7.58	8.81	8.33	9.96	7.24	4.26	10.84	4.82	5.68
x	10	8	13	9	11	14	6	4	12	7	5
y	9.14	8.14	8.47	8.77	9.26	8.10	6.13	3.10	9.13	7.26	4.74
x	8	8	8	8	8	8	8	8	8	8	19
y	6.58	5.76	7.71	8.84	8.47	7.04	5.25	5.56	7.91	6.89	12.50

t



Each of these data sets has a regression line $\hat{y} = 3 + 0.5x$ and correlations between 0.806 and 0.816. However, only the first is a suitable data set for linear regression. This example is meant to emphasize the point that software will happily compute a regression line and an r^2 value, but further examination of the data is required to see if this method is appropriate for any given data set.

3.3 Extensions

We will discuss briefly two extensions - the first is a least squares criterion between x and y that is **nonlinear** in the parameters $\beta = (\beta_0, \ldots, \beta_k)$. Thus, the model is

$$y_i = g(x_i|\beta) + \epsilon_i$$

for g, a nonlinear function of the parameters.

The second considers situations with more than one explanatory variable.

$$y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_k x_{ik} + \epsilon_i. \tag{3.20}$$

This brief discussion does not have the detail necessary to begin to use these methods. It serves primarily as an invitation to begin to consult resources that more fully develop these ideas.

3.3.1 Nonlinear Regression

Here, we continue using estimation of parameters using a **least squares** criterion.

$$SS(\beta) = \sum_{i=1}^{n} (y_i - g(x_i|\beta))^2.$$

For most choices of $g(x|\beta)$ the solution to the nonlinear least square criterion cannot be expressed in closed form. Thus, a numerical strategy for the solution $\hat{\beta}$ is necessary. This generally begins with some initial guess of parameter values and an iteration scheme to minimize $SS(\beta)$. Such a scheme is likely to use local information about the first and second partial derivatives of g with respect to the parameters β_i. For example, **gradient descent** (also known as **steepest descent**, or the **method of steepest descent**) is an iterative method in which produces a sequence of parameter values. The increment of the parameter values for an iteration is proportional to the negative of the gradient of $SS(\beta)$ evaluated at the current point. The hope is that the sequence converges to give the desired minimum value for $SS(\beta)$.

The R command `gnls` for **general nonlinear least squares** is used to accomplish this. As above, you should examine the residual plot to see that it has no structure. For, example, if the Lineweaver-Burke method for Michaelis-Mentens kinetics yields structure in the residuals, then linear regression is not considered a good method. Under these circumstances, one can next try to use the parameter estimates derived from Lineweaver-Burke as an initial guess in a nonlinear least squares regression using a least square criterion based on the sum of squares

$$SS(V_{max}, K_m) = \sum_{j=1}^{n} \left(V_j - V_{max} \frac{[S]_j}{K_m + [S]_j} \right)^2$$

for data $(V_1, [S]_1), (V_2, [S]_2), \ldots (V_n, [S]_n)$.

3.3.2 Multiple Linear Regression

Before we start with multiple linear regression, we first recall a couple of concepts and results from linear algebra.

- Let C_{ij} denote the entry in the i-th row and j-th column of a matrix C.

- A matrix A with r_A rows and c_A and a matrix B with r_B rows and c_B columns can be multiplied to form a matrix AB provide that $c_A = r_B$, the number of columns in A equals the number of rows in B. In this case

$$(AB)_{ij} = \sum_{k=1}^{c_A} A_{ik}B_{kj}.$$

- The d-dimensional **identity matrix** I is the matrix with the value 1 for all entries on the diagonal ($I_{jj} = 1, j = 1 \ldots, d$) and 0 for all other entries. Notice for and d-dimensional vector x,

$$Ix = x.$$

- A $d \times d$ matrix C is called invertible with **inverse** C^{-1} provided that

$$CC^{-1} = C^{-1}C = I.$$

  only one matrix can have this property.

- Suppose we have a d-dimensional vector a of known values and a $d \times d$ matrix C and we want to determine the vectors x that satisfy

$$a = Cx.$$

  This equation could have no solutions, a single solution, or an infinite number of solutions. If the matrix C is invertible, then we have a single solution

$$x = C^{-1}a.$$

- The **transpose** of a matrix is obtained by reversing the rows and columns of a matrix. We use a superscript T to indicate the transpose. Thus, the ij entry of a matrix C is the ji entry of its transpose, C^T.

  Example 3.23.

$$\begin{pmatrix} 2 & 1 & 3 \\ 4 & 2 & 7 \end{pmatrix}^T = \begin{pmatrix} 2 & 4 \\ 1 & 2 \\ 3 & 7 \end{pmatrix}$$

- A square matrix C is invertible if and only if its determinant $\det(C) \neq 0$. For a 2×2 matrix

$$C = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$$

  $\det(C) = ad - bc$ and the matrix inverse

$$C^{-1} = \frac{1}{\det(C)} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix}$$

Exercise 3.24. $(Cx)^T = x^T C^T$

Exercise 3.25. *For*

$$C = \begin{pmatrix} 1 & 3 \\ 2 & 4 \end{pmatrix},$$

find $\det(C)$ *and* C^{-1}.

In multiple linear regression, we have more than one predictor or explanatory random variable. Thus can write (3.20) in matrix form

$$y = X\beta + \epsilon \tag{3.21}$$

- $y = (y_1, y_2, \ldots, y_n)^T$ is a column vector of responses,
- X is a matrix of predictors,

$$X = \begin{pmatrix} 1 & x_{11} & \cdots & x_{1k} \\ 1 & x_{21} & \cdots & x_{2k} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & \cdots & x_{nk} \end{pmatrix}. \tag{3.22}$$

  The column of ones on the left give the constant term in a multilinear equation. This matrix X is an an example of what is know as a **design matrix**.

- $\beta = (\beta_0, \beta_1, \ldots, \beta_k)^T$ is a column vector of parameters, and
- $\epsilon = (\epsilon_1, \epsilon_2, \ldots, \epsilon_n)^T$ is a column vector of "errors".

Exercise 3.26. *Show that the least squares criterion*

$$SS(\beta) = \sum_{i=1}^{n} (y_i - \beta_0 - x_{i1}\beta_1 - \cdots - \beta_k x_{ik})^2. \tag{3.23}$$

can be written in matrix form as

$$SS(\beta) = (\mathbf{y} - X\beta)^T (\mathbf{y} - X\beta).$$

To minimize SS, we take the gradient and set it equal to 0.

Exercise 3.27. *Check that the gradient is*

$$\nabla_\beta SS(\beta) = -2(\mathbf{y} - X\beta)^T X. \tag{3.24}$$

Based on the exercise above, the value $\hat{\beta}$ that minimizes SS is

$$(\mathbf{y} - X\hat{\beta})^T X = 0, \quad \mathbf{y^T} X = \hat{\beta}^T X^T X.$$

Taking the transpose of this last equation

$$X^T X \hat{\beta} = X^T \mathbf{y}.$$

If $X^T X$ is invertible, then we can multiply both sides of the equation above by $(X^T X)^{-1}$ to obtain an equation for the parameter values $\hat{\beta} = (\hat{\beta}_0, \hat{\beta}_1, \ldots, \hat{\beta}_n)$ in the least squares regression.

$$\hat{\beta} = (X^T X)^{-1} X^T \mathbf{y}. \tag{3.25}$$

Thus the estimates $\hat{\beta}$ are a linear transformation of the repsonses $\mathbf{y}$ through the so-called **hat matrix** $H = (X^T X)^{-1} X^T$, i.e. $\hat{\beta} = H\mathbf{y}$.

Exercise 3.28. *Verify that the hat matrix H is a left inverse of the design matrix X.*

This gives the regression equation

$$y = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2 + \cdots + \hat{\beta}_k x_k$$

Example 3.29 (ordinary least squares regression)**.** *In this case,*

$$X^T X = \begin{pmatrix} 1 & 1 & \cdots & 1 \\ x_1 & x_2 & \cdots & x_n \end{pmatrix} \begin{pmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{pmatrix} = \begin{pmatrix} n & \sum_{i=1}^n x_i \\ \sum_{i=1}^n x_i & \sum_{i=1}^n x_i^2 \end{pmatrix}$$

and

$$X^T y = \begin{pmatrix} 1 & 1 & \cdots & 1 \\ x_1 & x_2 & \cdots & x_n \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} = \begin{pmatrix} \sum_{i=1}^n y_i \\ \sum_{i=1}^n x_i y_i \end{pmatrix}.$$

The determinant of $X^T X$ is

$$n\sum_{i=1}^n x_i^2 - \left(\sum_{i=1}^n x_i\right)^2 = n(n-1)\text{var}(x).$$

and thus

$$(X^T X)^{-1} = \frac{1}{n(n-1)\text{var}(x)} \begin{pmatrix} \sum_{i=1}^n x_i^2 & -\sum_{i=1}^n x_i \\ -\sum_{i=1}^n x_i & n \end{pmatrix}$$

and

$$\hat{\beta} = (X^T X)^{-1} X^T \mathbf{y} = \frac{1}{n(n-1)\text{var}(x)} \begin{pmatrix} \sum_{i=1}^n x_i^2 & -\sum_{i=1}^n x_i \\ -\sum_{i=1}^n x_i & n \end{pmatrix} \begin{pmatrix} \sum_{i=1}^n y_i \\ \sum_{i=1}^n x_i y_i \end{pmatrix}.$$

For example, for the second row, we obtain

$$\frac{1}{n(n-1)\text{var}(x)} \left(\left(-\sum_{i=1}^n x_i \right) \left(\sum_{i=1}^n y_i \right) + n \sum_{i=1}^n x_i y_i \right) = \frac{n(n-1)\text{cov}(x,y)}{n(n-1)\text{var}(x)} = \frac{\text{cov}(x,y)}{\text{var}(x)}$$

*as seen in equation (**??**).*

Example 3.30. *The choice of $x_{ij} = x_i^j$ in (3.22) results in* **polynomial regression**

$$y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \cdots + \beta_k x_i^k + \epsilon_i.$$

in equation (3.20).

Example 3.31 (US population)**.** *Below are the census populations*

year	census population	year	census population	year	census population	year	census population
1790	3,929,214	1850	23,191,876	1910	92,228,496	1970	203,211,926
1800	5,236,631	1860	31,443,321	1920	106,021,537	1980	226,545,805
1810	7,239,881	1870	38,558,371	1930	123,202,624	1990	248,709,873
1820	9,638,453	1880	49,371,340	1940	132,164,569	2000	281,421,906
1830	12,866,020	1890	62,979,766	1950	151,325,798	2010	308,745,538
1840	17,069,453	1900	76,212,168	1960	179,323,175		

To analyze this in R *we enter the data:*

```
> uspop<-c(3929214,5236631,7239881,9638453,12866020,17069453,23191876,31443321,
+ 38558371,49371340,62979766,76212168,92228496,106021537,123202624,132164569,
+ 151325798,179323175,203211926,226545805,248709873,281421906,308745538)
> year<-c(0:22)*10+1790
> plot(year,uspop)
> loguspop<-log(uspop,10)
> plot(year,loguspop)
```

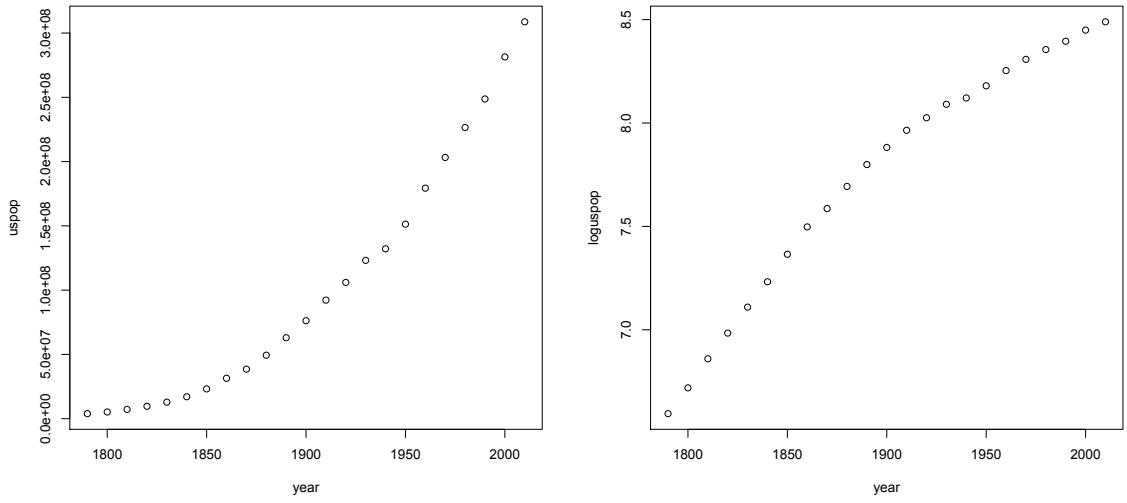


Figure 3.7: (a) United States census population from 1790 to 2010 and (b) its base 10 logarithm.

Note that the logarithm of the population still has a bend to it, so we will perform a quadratic regression on the logarithm of the population. In order to keep the numbers smaller, we shall give the year minus 1790, the year of the first census for our explanatory variable.

$$\log(uspopulation) = \beta_0 + \beta_1(year - 1790) + \beta_2(year - 1790)^2.$$

```
> year1<-year-1790
> year2<-year1^2
```

Thus, `loguspop` *is the reponse variable. The + sign is used in the case of more than one explanatory variable and here is placed between the response variables* `year1` *and* `year2`.

```
> lm.uspop<-lm(loguspop~year1+year2)
> summary(lm.uspop)

Call:
lm(formula = loguspop ~ year1 + year2)

Residuals:
      Min        1Q    Median        3Q       Max
-0.037387 -0.013453 -0.000912  0.015281  0.029782

Coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept)  6.582e+00  1.137e-02  578.99   <2e-16 ***
year1        1.471e-02  2.394e-04   61.46   <2e-16 ***
year2       -2.808e-05  1.051e-06  -26.72   <2e-16 ***
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1
```

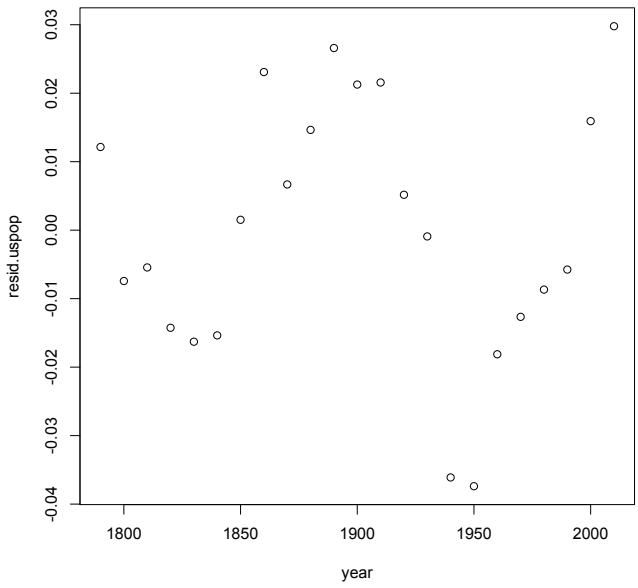


Figure 3.8: Residual plot for US population regression.

```
Residual standard error: 0.01978 on 20 degrees of freedom
Multiple R-squared: 0.999,Adjusted R-squared: 0.9989
F-statistic:  9781 on 2 and 20 DF,  p-value: < 2.2e-16
```

The R *output shows us that*

$$\hat{\beta}_0 = 6.587 \quad \hat{\beta}_1 = 0.1189 \quad \hat{\beta}_2 = -0.00002808.$$

So, taking the the regression line to the power 10, we have that

$$\widehat{uspopulation} = 3863670 \times 10^{0.1189(year-1790)-0.00002808(year-1790)^2}$$

In Figure 3.8, we show the residual plot for the logarithm of the US population.

```
> resid.uspop<-resid(lm.uspop)
> plot(year,resid.uspop)
```

3.4 Answers to Selected Exercises

3.1. Negative covariance means that the terms $(x_i - \bar{x})(y_i - \bar{y})$ in the sum are more likely to be negative than positive. This occurs whenever one of the x and y variables is above the mean, then the other is likely to be below.

3.2. We expand the product inside the sum.

$$\begin{aligned}\text{cov}(x,y) &= \frac{1}{n-1}\sum_{i=1}^{n}(x_i-\bar{x})(y_i-\bar{y}) = \frac{1}{n-1}\left(\sum_{i=1}^{n}x_iy_i - \bar{y}\sum_{i=1}^{n}x_i - \bar{x}\sum_{i=1}^{n}y_i + n\bar{x}\bar{y}\right)\\ &= \frac{1}{n-1}\left(\sum_{i=1}^{n}x_iy_i - n\bar{x}\bar{y} - n\bar{x}\bar{y} + n\bar{x}\bar{y}\right) = \frac{1}{n-1}\left(\sum_{i=1}^{n}x_iy_i - n\bar{x}\bar{y}\right)\end{aligned}$$

The change in measurements from centimeters to meters would divide the covariance by 10,000.

3.3. We rearrange the terms and simplify.

$$\begin{aligned}\text{cov}(ax+b,cy+d) &= \frac{1}{n-1}\sum_{i=1}^{n}((ax_i+b)-(a\bar{x}+b)((cy_i+d)-(c\bar{y}-d))\\ &= \frac{1}{n-1}\sum_{i=1}^{n}(ax_i-a\bar{x})(cy_i-c\bar{y}) = ac\cdot\frac{1}{n-1}\sum_{i=1}^{n}(x_i-\bar{x})(y_i-\bar{y}) = ac\cdot\text{cov}(x,y)\end{aligned}$$

3.5. Assume that $a \neq 0$ and $c \neq 0$. If $a = 0$ or $c = 0$, then the covariance is 0 and so is the correlation.

$$r(ax+b,cy+d) = \frac{\text{cov}(ax+b,cy+d)}{s_{ax+b}s_{cy+d}} = \frac{ac\cdot\text{cov}(x,y)}{|a|s_x\cdot|c|s_y} = \frac{ac}{|ac|}\frac{\cdot\text{cov}(x,y)}{s_x\cdot s_y} = \pm r(x,y)$$

We take the plus sign if the sign of a and c agree and the minus sign if they differ.

3.6. First we rearrange terms

$$\begin{aligned}s_{x+y}^2 &= \frac{1}{n-1}\sum_{i=1}^{n}((x_i+y_i)-(\bar{x}+\bar{y}))^2 = \frac{1}{n-1}\sum_{i=1}^{n}((x_i-\bar{x})+(y_i-\bar{y}))^2\\ &= \frac{1}{n-1}\sum_{i=1}^{n}(x_i-\bar{x})^2 + 2\frac{1}{n-1}\sum_{i=1}^{n}(x_i-\bar{x})(y_i-\bar{y}) + \frac{1}{n-1}\sum_{i=1}^{n}(y_i-\bar{y})^2\\ &= s_x^2 + 2\text{cov}(x,y) + s_y^2 = s_x^2 + 2rs_xs_y + s_y^2\end{aligned}$$

For a triangle with sides a, b and c, the law of cosines states that

$$c^2 = a^2 + b^2 - 2ab\cos\theta$$

where θ is the measure of the angle opposite side c. Thus the analogy is

s_x corresponds to a, s_y corresponds to b, s_{x+y} corresponds to c, and r corresponds to $-\cos\theta$

Notice that both r and $\cos\theta$ take values between -1 and 1.

3.7. Using the hint,

$$0 \leq \sum_{i=1}^{n}(v_i+w_i\zeta)^2 = \sum_{i=1}^{n}v_i^2 + 2\left(\sum_{i=1}^{n}v_iw_i\right)\zeta + \left(\sum_{i=1}^{n}w_i^2\right)\zeta^2 = A + B\zeta + C\zeta^2$$

For a quadratic equation to always take on non-negaitive values, we must have a non-positive discriminant, i. e.,

$$0 \geq B^2 - 4AC = 4\left(\sum_{i=1}^{n}v_iw_i\right)^2 - 4\left(\sum_{i=1}^{n}v_i^2\right)\left(\sum_{i=1}^{n}w_i^2\right).$$

Now, divide by 4 and rearrange terms.

$$\left(\sum_{i=1}^{n} v_i^2\right)\left(\sum_{i=1}^{n} w_i^2\right) \geq \left(\sum_{i=1}^{n} v_i w_i\right)^2.$$

3.8. The value of the correlation is the same for pairs of observations and for their standardized versions. Thus, we take x and y to be standardized observations. Then $s_x = s_y = 1$. Now, using equation (3.1), we have that

$0 \leq s_{x+y}^2 = 1 + 1 + 2r = 2 + 2r$. Simplifying, we have $-2 \leq 2r$ and $r \geq -1$.

For the second inequality, use the similar identity to (3.1) for the difference in the observations

$$s_{x-y}^2 = s_x^2 + s_y^2 - 2r s_x s_y.$$

Then,

$0 \leq s_{x-y} = 1 + 1 - 2r = 2 - 2r$. Simplifying, we have $2r \leq 2$ and $r \leq 1$.

Thus, correlation must always be between -1 and 1.

In the case that $r = -1$, we that that $s_{x+y}^2 = 0$ and thus using the standardized coordinates

$$\frac{x_i - \bar{x}}{s_x} + \frac{y_i - \bar{y}}{s_y} = 0.$$

Thus, $\zeta = s_y/s_x$.

In the case that $r = 1$, we that that $s_{x-y}^2 = 0$ and thus using the standardized coordinates

$$\frac{x_i - \bar{x}}{s_x} - \frac{y_i - \bar{y}}{s_y} = 0.$$

Thus, $\zeta = -s_y/s_x$.

3.10.

1. First the data and the scatterplot, preparing by using `mfrow`to have side-by-side plots

```
> x<-c(-2:3)
> y<-c(-3,-1,-2,0,4,2)
> par(mfrow=c(1,2))
> plot(x,y)
```

2. Then the regression line and its summary.

```
> regress.lm<-lm(y~x)
> summary(regress.lm)

Call:
lm(formula = y ~ x)

Residuals:
         1          2          3          4          5          6
-2.776e-16  8.000e-01 -1.400e+00 -6.000e-01  2.200e+00 -1.000e+00

Coefficients:
```

```
             Estimate Std. Error t value Pr(>|t|)
(Intercept)  -0.6000     0.6309  -0.951   0.3955
x             1.2000     0.3546   3.384   0.0277 *
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1

Residual standard error: 1.483 on 4 degrees of freedom
Multiple R-squared:  0.7412,Adjusted R-squared:  0.6765
F-statistic: 11.45 on 1 and 4 DF,  p-value: 0.02767
```

3. Add the regression line to the scatterplot.

```
> abline(regress.lm)
```

4. Make a data frame to show the predictions and the residuals.

```
> residuals<-resid(regress.lm)
> predictions<-predict(regress.lm,newdata=data.frame(x=c(-2:3)))
> data.frame(x,y,predictions,residuals)
   x  y predictions     residuals
1 -2 -3        -3.0 -2.775558e-16
2 -1 -1        -1.8  8.000000e-01
3  0 -2        -0.6 -1.400000e+00
4  1  0         0.6 -6.000000e-01
5  2  4         1.8  2.200000e+00
6  3  2         3.0 -1.000000e+00
```

5. FInally, the residual plot and a horizontal line at 0.

```
> plot(x,residuals)
> abline(h=0)
```

3.13. Use the subscript y in $\hat{\alpha}_y$ and $\hat{\beta}_y$ to emphasize that y is the explanatory variable. We still have $\bar{x} = 0.5, \bar{y} = 0$.

y_i	x_i	$y_i - \bar{y}$	$x_i - \bar{x}$	$(x_i - \bar{x})(y_i - \hat{y})$	$(y_i - \bar{y})^2$
-3	-2	-3	-2.5	7.5	9
-1	-1	-1	-1.5	1.5	1
-2	0	-2	-0.5	1.0	4
0	1	0	0.5	0.0	0
4	2	4	1.5	6.0	16
2	3	2	2.5	5.0	4
total		0	0	$\text{cov}(x, y) = 21/5$	$\text{var}(y) = 34/5$

So, the slope $\hat{\beta}_y = 21/34$ and

$$\bar{x} = \hat{\alpha}_y + \hat{\beta}_y \bar{y}, \quad 1/2 = \hat{\alpha}_y.$$

Thus, to predict x from y, the regression line is $\hat{x}_i = 1/2 + 21/34 y_i$. Because the product of the slopes

$$\frac{6}{5} \times \frac{21}{34} = \frac{63}{85} \neq 1,$$

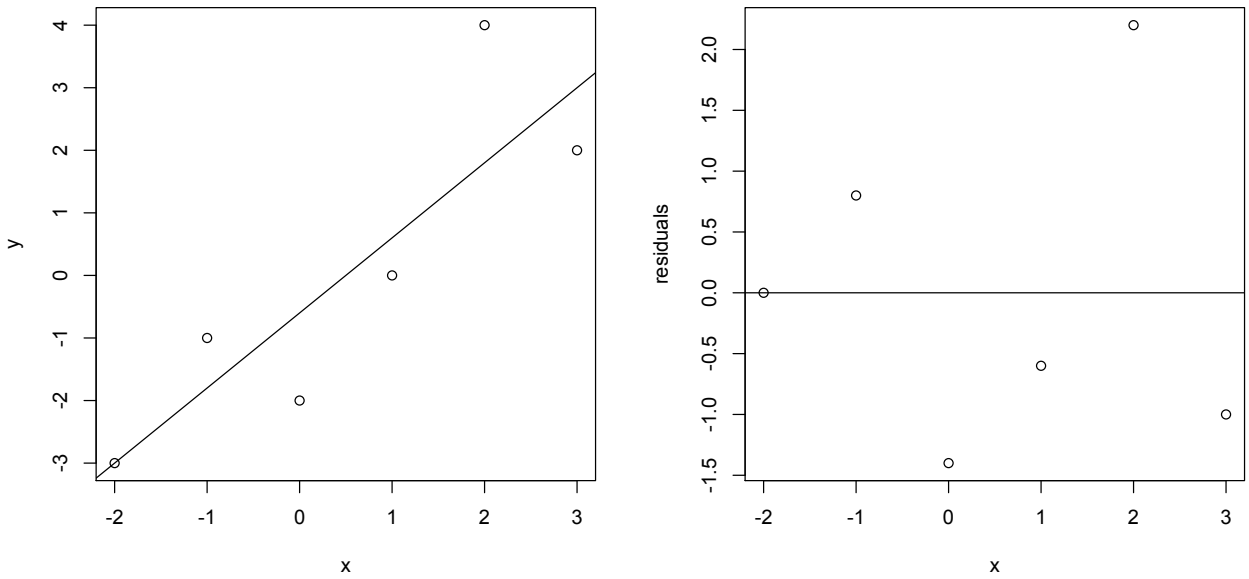


Figure 3.9: (left) scatterplot and regression line (right) residual plot and horizontal line at 0

this line differs from the line used to predict y from x.

3.14. Recall that the covariance of x and y is symmetric, i.e., $\text{cov}(x, y) = \text{cov}(y, x)$. Thus,

$$\hat{\beta}_x \cdot \hat{\beta}_y = \frac{\text{cov}(x,y)}{s_x^2} \cdot \frac{\text{cov}(y,x)}{s_y^2} = \frac{\text{cov}(x,y)^2}{s_x^2 s_y^2} = \left(\frac{\text{cov}(x,y)}{s_x s_y}\right)^2 = r^2.$$

In the example above,

$$r^2 = \frac{\text{cov}(x,y)^2}{s_x^2 x_y^2} = \frac{(21/5)^2}{(17.5/5)\cdot(34/5)} = \frac{21^2}{17.5 \cdot 34} = \frac{21}{35} \cdot \frac{21}{17} = \frac{3}{5} \cdot \frac{21}{17} = \frac{63}{85}$$

3.15 To show that the correlation is zero, we show that the numerator in the definition, the covariance is zero. First,

$$\text{cov}(\hat{y}, y - \hat{y}) = \text{cov}(\hat{y}, y) - \text{cov}(\hat{y}, \hat{y}).$$

The first term in this difference,

$$\text{cov}(\hat{y}, y) = \text{cov}\left(\frac{\text{cov}(x,y)}{s_x^2} x, y\right) = \frac{\text{cov}(x,y)^2}{s_x^2} = \frac{r^2 s_x^2 s_y^2}{s_x^2} = r^2 s_y^2.$$

For the second,

$$\text{cov}(\hat{y}, \hat{y}) = s_{\hat{y}}^2 = r^2 s_y^2.$$

So, the difference is 0.

3.16. For the denominator

$$s_{DATA}^2 = \frac{1}{n-1} \sum_{i=1}^{n} (y_i - \bar{y})^2$$

For the numerator, recall that $(\bar{x}, \bar{y})$ is on the regression line. Consequently, $\bar{y} = \hat{\alpha} + \hat{\beta}\bar{x}$. Thus, the mean of the fits

$$\bar{\hat{y}} = \frac{1}{n}\sum_{i=1}^{n} \hat{y}_i = \frac{1}{n}\sum_{i=1}^{n}(\hat{\alpha} + \hat{\beta}x_i) = \hat{\alpha} + \hat{\beta}\bar{x} = \bar{y}.$$

This could also be seen by using the fact (3.11) that the sum of the residuals is 0. For the denominator,

$$s^2_{FIT} = \frac{1}{n-1}\sum_{i=1}^{n}(\hat{y}_i - \bar{\hat{y}})^2 = \frac{1}{n-1}\sum_{i=1}^{n}(\hat{y}_i - \bar{y})^2.$$

Now, take the ratio and notice that the fractions $1/(n-1)$ in the numerator and denominator cancel.

3.17. The least squares criterion becomes

$$S(\beta) = \sum_{i=1}^{n}(y_i - \beta x_i)^2.$$

The derivative with respect to β is

$$S'(\beta) = -2\sum_{i=1}^{n} x_i(y_i - \beta x_i).$$

$S'(\beta) = 0$ for the value

$$\hat{\beta} = \frac{\sum_{i=1}^{n} x_i y_i}{\sum_{i=1}^{n} x_i^2}.$$

3.21. The i-th component of $(Cx)^T$ is

$$\sum_{j=1}^{n} C_{ij}x_j.$$

Now the i-th component of $x^T C^T$ is

$$\sum_{j=1}^{n} x_j C^T_{ji} = \sum_{j=1}^{n} x_j C_{ij}.$$

3.24. $\det(C) = 4 - 6 = -2$ and

$$C^{-1} = \frac{1}{-2}\begin{pmatrix} 4 & -3 \\ -2 & 1 \end{pmatrix} = \begin{pmatrix} -2 & 3/2 \\ 1 & -1/2 \end{pmatrix}.$$

3.25. Using equation (3.21), the i-th component of $\mathbf{y} - X\beta$,

$$(\mathbf{y} - X\beta)_i = y_i - \sum_{j=0}^{n} \beta_j x_{jk} = y_i - \beta_0 - x_{i1}\beta_1 - \cdots - \beta_k x_{in}.$$

Now, $(\mathbf{y} - X\beta)^T(\mathbf{y} - X\beta)$ is the dot product of $\mathbf{y} - X\beta$ with itself. This gives (3.23).

3.26. Write $x_{i0} = 1$ for all i, then we can write (3.23) as

$$SS(\beta) = \sum_{i=1}^{n}(y_i - x_{i0}\beta_0 - x_{i1}\beta_1 - \cdots - \beta_k x_{ik})^2.$$

Then,

$$\begin{aligned}\frac{\partial}{\partial \beta_j} S(\beta) &= -2\sum_{i=1}^{n}(y_i - x_{i0}\beta_0 - x_{i1}\beta_1 - \cdots - \beta_k x_{ik})x_{ij} \\ &= -2\sum_{i=1}^{n}(y_i - (X\beta)_i)x_{ij} = -2((y - X\beta)^T X))_j.\end{aligned}$$

This is the j-th coordinate of (3.24).

3.27. $HX = (X^TX)^{-1}X^TX = (X^TX)^{-1}(X^TX) = I$, the identity matrix.