Statistical Methods II

Derek L. Sonderegger

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Chapter 1

Matrix Theory

Almost all of the calculations done in classical statistics require formulas with large number of subscripts and many different sums. In this chapter we will develop the mathematical machinery to write these formulas in a simple compact formula using *matrices*.

1.1 Types of Matrices

We will first introduce the idea behind a matrix and give several special types of matrices that we will encounter.

1.1.1 Scalars

To begin, we first define a *scalar*. A scalar is just a single number, either real or complex. The key is that a scalar is just a single number. For example, 6 is a scalar, as is -3. By convention, variable names for scalars will be lower case and not in bold typeface.

Examples could be $a = 5$, $b = \sqrt{3}$, or $\sigma = 2$.

1.1.2 Vectors

A vector is collection of scalars, arranged as a row or column. Our convention will be that a vector will be a lower cased letter but written in a bold type. In other branches of mathematics is common to put a bar over the variable name to denote that it is a vector, but in statistics, we have already used a bar to denote a mean.

Examples of column vectors could be

$$\boldsymbol{a} = \begin{bmatrix} 2 \\ -3 \\ 4 \end{bmatrix} \quad \boldsymbol{b} = \begin{bmatrix} 2 \\ 8 \\ 3 \\ 4 \\ 1 \end{bmatrix}$$

and examples of row vectors are

$$\boldsymbol{c} = \begin{bmatrix} 8 & 10 & 43 & -22 \end{bmatrix}$$

$$\boldsymbol{d} = \begin{bmatrix} -1 & 5 & 2 \end{bmatrix}$$

To denote a specific entry in the vector, we will use a subscript. For example, the second element of $\boldsymbol{d}$ is $d_2 = 5$. Notice, that we do not bold this symbol because the second element of the vector is the scalar value 5.

1.1.3 Matrix

Just as a vector is a collection of scalars, a matrix can be viewed as a collection of vectors (all of the same length). We will denote matrices with bold capitalized letters. In general, I try to use letters at the end of the alphabet for matrices. Likewise, I try to use symmetric letters to denote symmetric matrices.

For example, the following is a matrix with two rows and three columns

$$\boldsymbol{W} = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{bmatrix}$$

and there is no requirement that the number of rows be equal, less than, or greater than the number of columns. In denoting the size of the matrix, we first refer to the number of rows and then the number of columns. Thus $\boldsymbol{W}$ is a 2×3 matrix and it sometimes is helpful to remind ourselves of this by writing $\boldsymbol{W}_{2\times 3}$.

To pick out a particular element of a matrix, I will again use a subscripting notation, always with the row number first and then column. Notice the notational shift to lowercase, non-bold font.

$$w_{1,2} = 2 \qquad \text{and} \qquad w_{2,3} = 6$$

There are times I will wish to refer to a particular row or column of a matrix and we will use the following notation

$$\boldsymbol{w}_{1,\cdot} = \begin{bmatrix} 1 & 2 & 3 \end{bmatrix}$$

is the first row of the matrix $\boldsymbol{W}$. The second column of matrix $\boldsymbol{W}$ is

$$\boldsymbol{w}_{\cdot,2} = \begin{bmatrix} 2 \\ 5 \end{bmatrix}$$

1.1.4 Square Matrices

A square matrix is a matrix with the same number of rows as columns. The following are square

$$\boldsymbol{Z} = \begin{bmatrix} 3 & 6 \\ 8 & 10 \end{bmatrix} \qquad \boldsymbol{X} = \begin{bmatrix} 1 & 2 & 3 \\ 2 & 1 & 2 \\ 3 & 2 & 1 \end{bmatrix}$$

1.1.5 Symmetric Matrices

In statistics we are often interested in square matrices where the i, j element is the same as the j, i element. For example, $x_{1,2} = x_{2,1}$ in the above matrix $\boldsymbol{X}$.

Consider a matrix $\boldsymbol{D}$ that contains the distance from four towns to each of the other four towns. Let $d_{i,j}$ be the distance from town i to town j. It only makes sense that the distance doesn't matter which direction you are traveling, and we should therefore require that $d_{i,j} = d_{j,i}$.

In this example, it is the values $d_{i,i}$ represent the distance from a town to itself, which should be zero. It turns out that we are often interested in the terms $d_{i,i}$ and I will refer to those terms as the *main diagonal* of matrix $\boldsymbol{D}$.

Symmetric matrices play a large role in statistics because matrices that represent the covariances between random variables must be symmetric because $Cov(Y, Z) = Cov(Z, Y)$.

1.1.6 Diagonal Matrices

A square matrix that has zero entries in every location except the main diagonal is called a diagonal matrix. Here are two examples:

$$\boldsymbol{Q} = \begin{bmatrix} 4 & 0 & 0 \\ 0 & 5 & 0 \\ 0 & 0 & 6 \end{bmatrix} \qquad \boldsymbol{R} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 3 \end{bmatrix}$$

Sometimes to make matrix more clear, I will replace the 0 with a dot to emphasize the non-zero components.

$$\boldsymbol{R} = \begin{bmatrix} 1 & \cdot & \cdot & \cdot \\ \cdot & 2 & \cdot & \cdot \\ \cdot & \cdot & 2 & \cdot \\ \cdot & \cdot & \cdot & 3 \end{bmatrix}$$

1.1.7 Identity Matrices

A diagonal matrix with main diagonal values exactly 1 is called the identity matrix. The 3×3 identity matrix is denoted I_3.

$$\boldsymbol{I}_3 = \begin{bmatrix} 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \end{bmatrix}$$

1.2 Operations on Matrices

1.2.1 Transpose

The simplest operation on a square matrix matrix is called *transpose*. It is defined as $\boldsymbol{M} = \boldsymbol{W}^T$ if and only if $m_{i,j} = w_{j,i}$.

$$\boldsymbol{Z} = \begin{bmatrix} 1 & 6 \\ 8 & 3 \end{bmatrix} \qquad \boldsymbol{Z}^T = \begin{bmatrix} 1 & 8 \\ 6 & 3 \end{bmatrix}$$

$$\boldsymbol{M} = \begin{bmatrix} 3 & 1 & 2 \\ 9 & 4 & 5 \\ 8 & 7 & 6 \end{bmatrix} \qquad \boldsymbol{M}^T = \begin{bmatrix} 3 & 9 & 8 \\ 1 & 4 & 7 \\ 2 & 5 & 6 \end{bmatrix}$$

We can think of this as swapping all elements about the main diagonal.

1.2.2 Addition and Subtraction

Addition and subtraction are performed *element-wise*. This means that two matrices or vectors can only be added or subtracted if their dimensions match.

$$\begin{bmatrix} 1 \\ 2 \\ 3 \\ 4 \end{bmatrix} + \begin{bmatrix} 5 \\ 6 \\ 7 \\ 8 \end{bmatrix} = \begin{bmatrix} 6 \\ 8 \\ 10 \\ 12 \end{bmatrix}$$

$$\begin{bmatrix} 5 & 8 \\ 2 & 4 \\ 11 & 15 \end{bmatrix} - \begin{bmatrix} 1 & 2 \\ 3 & 4 \\ 5 & -6 \end{bmatrix} = \begin{bmatrix} 4 & 6 \\ -1 & 0 \\ 6 & 21 \end{bmatrix}$$

1.2.3 Multiplication

Multiplication is the operation that is vastly different for matrices and vectors than it is for scalars. There is a great deal of mathematical theory that suggests a useful way to define multiplication. What is presented below is referred to as the *dot-product* of vectors in calculus, and is referred to as the standard *inner-product* in linear algebra.

1.2.4 Vector Multiplication

We first define multiplication for a row and column vector. For this multiplication to be defined, both vectors must be the same length. The product is the sum of the element-wise multiplications.

$$\begin{bmatrix} 1 & 2 & 3 & 4 \end{bmatrix} \begin{bmatrix} 5 \\ 6 \\ 7 \\ 8 \end{bmatrix} = (1 \cdot 5) + (2 \cdot 6) + (3 \cdot 7) + (4 \cdot 8) = 5 + 12 + 21 + 32 = 70$$

1.2.5 Matrix Multiplication

Matrix multiplication is just a sequence of vector multiplications. If $\boldsymbol{X}$ is a $m \times n$ matrix and $\boldsymbol{W}$ is $n \times p$ matrix then $\boldsymbol{Z} = \boldsymbol{XW}$ is a $m \times p$ matrix where $z_{ij} = \boldsymbol{x}_{i\cdot}\boldsymbol{w}_{\cdot j}$ where $\boldsymbol{x}_{i\cdot}$ is the ith column of $\boldsymbol{X}$ and $\boldsymbol{w}_{\cdot j}$ is the jth column of $\boldsymbol{W}$. For example, let

$$\boldsymbol{X} = \begin{bmatrix} 1 & 2 & 3 & 4 \\ 5 & 6 & 7 & 8 \\ 9 & 10 & 11 & 12 \end{bmatrix} \qquad \boldsymbol{W} = \begin{bmatrix} 13 & 14 \\ 15 & 16 \\ 17 & 18 \\ 19 & 20 \end{bmatrix}$$

so $\boldsymbol{X}$ is 3×4 (which we remind ourselves by adding a 3×4 subscript to $\boldsymbol{X}$ as $\boldsymbol{X}_{3\times4}$) and $\boldsymbol{W}$ is $\boldsymbol{W}_{4\times2}$. Because the *inner* dimensions match for this multiplication, then $\boldsymbol{Z}_{3\times2} = \boldsymbol{X}_{3\times4}\boldsymbol{W}_{4\times2}$ is defined where

$$\begin{aligned} z_{11} &= \boldsymbol{x}_{1\cdot}\boldsymbol{w}_{\cdot1} \\ &= (1 \cdot 13) + (2 \cdot 15) + (3 \cdot 17) + (4 \cdot 19) = 170 \end{aligned}$$

and similarly

$$\begin{aligned} z_{21} &= \boldsymbol{x}_{2\cdot}\boldsymbol{w}_{\cdot1} \\ &= (5 \cdot 13) + (6 \cdot 15) + (7 \cdot 17) + (8 \cdot 19) = 426 \end{aligned}$$

so that

$$\boldsymbol{Z} = \begin{bmatrix} 170 & 180 \\ 426 & 452 \\ 682 & 724 \end{bmatrix}$$

For another example, we note that

$$\begin{aligned} \begin{bmatrix} 1 & 2 & 3 \\ 2 & 3 & 4 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ 2 & 2 \\ 1 & 2 \end{bmatrix} &= \begin{bmatrix} 1+4+3 & 2+4+6 \\ 2+6+4 & 4+6+8 \end{bmatrix} \\ &= \begin{bmatrix} 8 & 12 \\ 12 & 18 \end{bmatrix} \end{aligned}$$

Notice that this definition of multiplication means that the order matters. Above, we calculated $\boldsymbol{X}_{3\times4}\boldsymbol{W}_{4\times2}$ but we cannot reverse the order because the inner dimensions do not match up.

1.2.6 Scalar times a Matrix

Strictly speaking, we are not allowed to multiply a matrix by a scalar because the dimensions do not match. However, it is often notationally convenient. So we define $a\boldsymbol{X}$ to be the *element-wise* multiplication of each element of $\boldsymbol{X}$ by the scalar a. Because this is just a notational convenience, the mathematical theory about inner-products does not apply to this operation.

$$5\begin{bmatrix} 4 & 5 \\ 7 & 6 \\ 9 & 10 \end{bmatrix} = \begin{bmatrix} 20 & 25 \\ 35 & 30 \\ 45 & 50 \end{bmatrix}$$

Because of this definition, it is clear that $a\boldsymbol{X} = \boldsymbol{X}a$ and the order does not matter. Thus when mixing scalar multiplication with matrices, it is acceptable to reorder scalars, but not matrices.

1.2.7 Determinant

The determinant is defined only for square matrices and can be thought of as the matrix equivalent of the absolute value or magnitude (i.e. $|-6| = 6$). The determinant gives a measure of the multi-dimensional size of a matrix (say the matrix $\boldsymbol{A}$) and as such is denoted $\det(\boldsymbol{A})$ or $|\boldsymbol{A}|$. Generally this is a very tedious thing to calculate by hand and for completeness sake, we will give a definition and small examples.

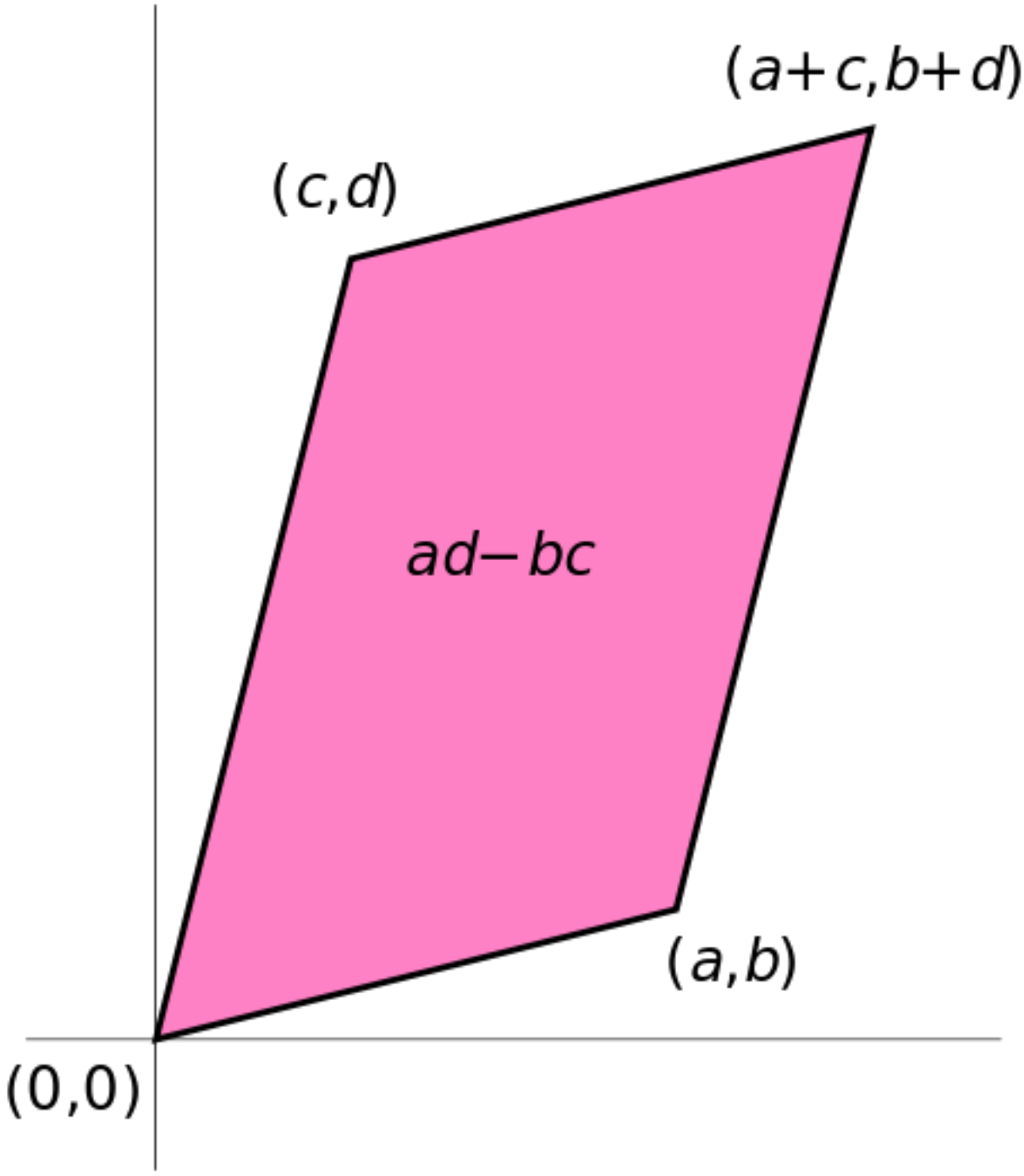
For a 2×2 matrix

$$\begin{vmatrix} a & c \\ b & d \end{vmatrix} = ad - cb$$

So a simple example of a determinant is

$$\begin{vmatrix} 5 & 2 \\ 3 & 10 \end{vmatrix} = 50 - 6 = 44$$

The determinant can be thought of as the area of the parallelogram created by the row or column vectors of the matrix.



1.2.8 Inverse

In regular algebra, we are often interested in solving equations such as

$$5x = 15$$

for x. To do so, we multiply each side of the equation by the inverse of 5, which is 1/5.

$$\begin{aligned} 5x &= 15 \\ \frac{1}{5} \cdot 5 \cdot x &= \frac{1}{5} \cdot 15 \\ 1 \cdot x &= 3 \\ x &= 3 \end{aligned}$$

For scalars, we know that the inverse of scalar a is the value that when multiplied by a is 1. That is we see to find a^{-1} such that $aa^{-1} = 1$.

In the matrix case, I am interested in finding $\boldsymbol{A}^{-1}$ such that $\boldsymbol{A}^{-1}\boldsymbol{A} = \boldsymbol{I}$ and $\boldsymbol{A}\boldsymbol{A}^{-1} = \boldsymbol{I}$. For both of these multiplications to be defined, $\boldsymbol{A}$ must be a square matrix and so the inverse is only defined for square matrices.

For a 2×2 matrix

$$\boldsymbol{W} = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$$

the inverse is given by:

$$\boldsymbol{W}^{-1} = \frac{1}{\det \boldsymbol{W}} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix}$$

For example, suppose

$$\boldsymbol{W} = \begin{bmatrix} 1 & 2 \\ 5 & 3 \end{bmatrix}$$

then $\det W = 3 - 10 = -7$ and

$$\begin{aligned} \boldsymbol{W}^{-1} &= \frac{1}{-7} \begin{bmatrix} 3 & -2 \\ -5 & 1 \end{bmatrix} \\ &= \begin{bmatrix} -\frac{3}{7} & \frac{2}{7} \\ \frac{5}{7} & -\frac{1}{7} \end{bmatrix} \end{aligned}$$

and thus

$$\begin{aligned} \boldsymbol{W}\boldsymbol{W}^{-1} &= \begin{bmatrix} 1 & 2 \\ 5 & 3 \end{bmatrix} \begin{bmatrix} -\frac{3}{7} & \frac{2}{7} \\ \frac{5}{7} & -\frac{1}{7} \end{bmatrix} \\ &= \begin{bmatrix} -\frac{3}{7} + \frac{10}{7} & \frac{2}{7} - \frac{2}{7} \\ -\frac{15}{7} + \frac{15}{7} & \frac{10}{7} - \frac{3}{7} \end{bmatrix} \\ &= \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \boldsymbol{I}_2 \end{aligned}$$

Not every square matrix has an inverse. If the determinant of the matrix (which we think of as some measure of the magnitude or *size* of the matrix) is zero, then the formula would require us to divide by zero. Just as we cannot find the inverse of zero (i.e. solve $0x = 1$ for x), a matrix with zero determinate is said to have no inverse.

1.3 Exercises

Consider the following matrices:

$$\mathbf{A} = \begin{bmatrix} 1 & 2 & 3 \\ 6 & 5 & 4 \end{bmatrix} \qquad \mathbf{B} = \begin{bmatrix} 6 & 4 & 3 \\ 8 & 7 & 6 \end{bmatrix} \qquad \mathbf{c} = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} \qquad \mathbf{d} = \begin{bmatrix} 4 \\ 5 \\ 6 \end{bmatrix} \qquad \mathbf{E} = \begin{bmatrix} 1 & 2 \\ 2 & 6 \end{bmatrix}$$

1. Find $\mathbf{Bc}$
2. Find $\mathbf{AB}^T$
3. Find $\mathbf{c}^T\mathbf{d}$
4. Find $\mathbf{cd}^T$
5. Confirm that $\mathbf{E}^{-1} = \begin{bmatrix} 3 & -1 \\ -1 & 1/2 \end{bmatrix}$ is the inverse of $\mathbf{E}$ by calculating $\mathbf{EE}^{-1} = \mathbf{I}$.

Chapter 2

Parameter Estimation

We have previously looked at ANOVA and regression models and, in many ways, they felt very similar. In this chapter we will introduce the theory that allows us to understand both models as a particular flavor of a larger class of models known as *linear models.*

First we clarify what a linear model is. A linear model is a model where the data (which we will denote using roman letters as $\boldsymbol{x}$ and $\boldsymbol{y}$) and parameters of interest (which we denote using greek letters such as $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$) interact only via addition and multiplication. The following are linear models:

Model	Formula
ANOVA	$y_{ij} = \mu + \tau_i + \epsilon_i$
Simple Regression	$y_i = \beta_0 + \beta_1 x_i + \epsilon_i$
Quadratic Term	$y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \epsilon_i$
General Regression	$y_i = \beta_0 + \beta_1 x_{i,1} + \beta_2 x_{i,2} + \cdots + \beta_p x_{i,p} + \epsilon_i$

Notice in the Quadratic model, the square is not a parameter and we can consider x_i^2 as just another column of data. This leads to the second example of multiple regression where we just add more slopes for other covariates where the p^{th} covariate is denoted $\boldsymbol{x}_{\cdot,p}$ and might be some transformation (such as x^2 or $\log x$) of another column of data. The critical point is that the transformation to the data $\boldsymbol{x}$ does not depend on a parameter. Thus the following is *not* a linear model

$$y_i = \beta_0 + \beta_1 x_i^{\alpha} + \epsilon_i$$

2.1 Simple Regression

We would like to represent all linear models in a similar compact matrix representation. This will allow us to make the transition between simple and multiple regression (and ANCOVA) painlessly.

To begin, we think about how to write the simple regression model using matrices and vectors that correspond the the data and the parameters. Notice we have

$$\begin{aligned} y_1 &= \beta_0 + \beta_1 x_1 + \epsilon_1 \\ y_2 &= \beta_0 + \beta_1 x_2 + \epsilon_2 \\ y_3 &= \beta_0 + \beta_1 x_3 + \epsilon_3 \\ &\vdots \\ y_{n-1} &= \beta_0 + \beta_1 x_{n-1} + \epsilon_{n-1} \\ y_n &= \beta_0 + \beta_1 x_n + \epsilon_n \end{aligned}$$

where, as usual, $\epsilon_i \overset{iid}{\sim} N\left(0, \sigma^2\right)$. These equations can be written using matrices as

$$\underbrace{\begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_{n-1} \\ y_n \end{bmatrix}}_{\boldsymbol{y}} = \underbrace{\begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ 1 & x_3 \\ \vdots & \vdots \\ 1 & x_{n-1} \\ 1 & x_n \end{bmatrix}}_{\boldsymbol{X}} \underbrace{\begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix}}_{\boldsymbol{\beta}} + \underbrace{\begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \epsilon_3 \\ \vdots \\ \epsilon_{n-1} \\ \epsilon_n \end{bmatrix}}_{\boldsymbol{\epsilon}}$$

and we compactly write the model as

$$\boldsymbol{y} = \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$$

where $\boldsymbol{X}$ is referred to as the *design matrix* and $\boldsymbol{\beta}$ is the vector of *location parameters* we are interested in estimating.

2.1.1 Estimation of Location Paramters

Our next goal is to find the best estimate of $\boldsymbol{\beta}$ given the data. To justify the formula, consider the case where there is no error terms (i.e. $\epsilon_i = 0$ for all i). Thus we have

$$\boldsymbol{y} = \boldsymbol{X}\boldsymbol{\beta}$$

and our goal is to solve for $\boldsymbol{\beta}$. To do this, we must use a matrix inverse, but since inverses only exist for square matrices, we pre-multiple by $\boldsymbol{X}^T$ (notice that $\boldsymbol{X}^T\boldsymbol{X}$ is a symmetric 2×2 matrix).

$$\boldsymbol{X}^T\boldsymbol{y} = \boldsymbol{X}^T\boldsymbol{X}\boldsymbol{\beta}$$

and then pre-multiply by $\left(\boldsymbol{X}^T\boldsymbol{X}\right)^{-1}$.

$$\begin{aligned} \left(\boldsymbol{X}^T\boldsymbol{X}\right)^{-1}\boldsymbol{X}^T\boldsymbol{y} &= \left(\boldsymbol{X}^T\boldsymbol{X}\right)^{-1}\boldsymbol{X}^T\boldsymbol{X}\boldsymbol{\beta} \\ \left(\boldsymbol{X}^T\boldsymbol{X}\right)^{-1}\boldsymbol{X}^T\boldsymbol{y} &= \boldsymbol{\beta} \end{aligned}$$

This exercise suggests that $\left(\boldsymbol{X}^T\boldsymbol{X}\right)^{-1}\boldsymbol{X}^T\boldsymbol{y}$ is a good place to start when looking for the maximum-likelihood estimator for $\boldsymbol{\beta}$. It turns out that this quantity is in fact the maximum-likelihood estimator (and equivalently minimizes the sum-of-squared error). Therefore we will use it as our estimate of $\boldsymbol{\beta}$.

$$\hat{\boldsymbol{\beta}} = \left(\boldsymbol{X}^T\boldsymbol{X}\right)^{-1}\boldsymbol{X}^T\boldsymbol{y}$$

2.1.2 Estimation of Variance Parameter

Recall our model is

$$y_i = \beta_0 + \beta_1 x_i + \epsilon_i$$

where $\epsilon_i \overset{iid}{\sim} N\left(0, \sigma^2\right)$. As usual we will find estimates of the noise terms (which we will call residuals or errors) via

$$\begin{aligned} \hat{\epsilon}_i &= y_i - \hat{y}_i \\ &= y_i - \left(\hat{\beta}_0 + \hat{\beta}_1 x_i\right) \end{aligned}$$

Writing $\hat{\boldsymbol{y}}$ in matrix terms we have

$$\begin{aligned} \hat{\boldsymbol{y}} &= \boldsymbol{X}\hat{\boldsymbol{\beta}} \\ &= \boldsymbol{X}\left(\boldsymbol{X}^T\boldsymbol{X}\right)^{-1}\boldsymbol{X}^T\boldsymbol{y} \\ &= \boldsymbol{H}\boldsymbol{y} \end{aligned}$$

where $\boldsymbol{H} = \boldsymbol{X}\left(\boldsymbol{X}^T\boldsymbol{X}\right)^{-1}\boldsymbol{X}^T$ is often called the *hat-matrix* because it takes y to $\hat{y}$ and has many interesting theoretical properties.[1]

We can now estimate the error terms via

$$\begin{aligned} \hat{\boldsymbol{\epsilon}} &= \boldsymbol{y} - \hat{\boldsymbol{y}} \\ &= \boldsymbol{y} - \boldsymbol{H}\boldsymbol{y} \\ &= \left(\boldsymbol{I}_n - \boldsymbol{H}\right)\boldsymbol{y} \end{aligned}$$

As usual we estimate σ^2 using the mean-squared error

$$\begin{aligned} \hat{\sigma}^2 &= \frac{1}{n-2}\sum_{i=1}^{n}\hat{\epsilon}_i^2 \\ &= \frac{1}{n-2}\,\hat{\boldsymbol{\epsilon}}^T\hat{\boldsymbol{\epsilon}} \end{aligned}$$

In the general linear model case where $\boldsymbol{\beta}$ has p elements (and thus we have $n-p$ degrees of freedom), the formula is

$$\hat{\sigma}^2 = \frac{1}{n-p}\,\hat{\boldsymbol{\epsilon}}^T\hat{\boldsymbol{\epsilon}}$$

[1] Mathematically, $\boldsymbol{H}$ is the projection matrix that takes a vector in n-dimensional space and projects it onto a p-dimension subspace spanned by the vectors in $\boldsymbol{X}$. Projection matrices have many useful properties and much of the theory of linear models utilizes $\boldsymbol{H}$.

2.1.3 Expectation and variance of a random vector

Just as we needed to derive the expected value and variance of $\bar{x}$ in the previous semester, we must now do the same for $\hat{\boldsymbol{\beta}}$. But to do this, we need some properties of expectations and variances.

In the following, let $\boldsymbol{A}_{n\times p}$ and $\boldsymbol{b}_{n\times 1}$ be constants and $\boldsymbol{\epsilon}_{n\times 1}$ be a random vector.

Expectations are very similar to the scalar case where

$$E\left[\boldsymbol{\epsilon}\right] = \begin{bmatrix} E\left[\epsilon_1\right] \\ E\left[\epsilon_2\right] \\ \vdots \\ E\left[\epsilon_n\right] \end{bmatrix}$$

and any constants are pulled through the expectation

$$E\left[\boldsymbol{A}^T\boldsymbol{\epsilon} + \boldsymbol{b}\right] = \boldsymbol{A}^T E\left[\epsilon\right] + \boldsymbol{b}$$

Variances are a little different. The variance of the vector $\boldsymbol{\epsilon}$ is

$$Var\left(\boldsymbol{\epsilon}\right) = \begin{bmatrix} Var\left(\epsilon_1\right) & Cov\left(\epsilon_1,\epsilon_2\right) & \dots & Cov\left(\epsilon_1,\epsilon_n\right) \\ Cov\left(\epsilon_2,\epsilon_1\right) & Var\left(\epsilon_2\right) & \dots & Cov\left(\epsilon_2,\epsilon_n\right) \\ \vdots & \vdots & \ddots & \vdots \\ Cov\left(\epsilon_n,\epsilon_1\right) & Cov\left(\epsilon_n,\epsilon_2\right) & \dots & Var\left(\epsilon_1\right) \end{bmatrix}$$

and additive constants are ignored, but multiplicative constants are pulled out as follows:

$$Var\left(\boldsymbol{A}^T\boldsymbol{\epsilon} + \boldsymbol{b}\right) = Var\left(\boldsymbol{A}^T\boldsymbol{\epsilon}\right) = \boldsymbol{A}^T Var\left(\boldsymbol{\epsilon}\right)\, \boldsymbol{A}$$

2.1.4 Variance of Location Parameters

We next derive the sampling variance of our estimator $\hat{\boldsymbol{\beta}}$ by first noting that $\boldsymbol{X}$ and $\boldsymbol{\beta}$ are constants and therefore

$$\begin{aligned} Var\left(\boldsymbol{y}\right) &= Var\left(\boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}\right) \\ &= Var\left(\boldsymbol{\epsilon}\right) \\ &= \sigma^2\boldsymbol{I}_n \end{aligned}$$

because the error terms are independent and therefore $Cov\left(\epsilon_i,\epsilon_j\right) = 0$ when $i \neq j$ and $Var\left(\epsilon_i\right) = \sigma^2$. Recalling that constants come out of the variance operator as the constant *squared,*

$$\begin{aligned} Var\left(\hat{\boldsymbol{\beta}}\right) &= Var\left(\left(\boldsymbol{X}^T\boldsymbol{X}\right)^{-1}\boldsymbol{X}^T\boldsymbol{y}\right) \\ &= \left(\boldsymbol{X}^T\boldsymbol{X}\right)^{-1}\boldsymbol{X}^T Var\left(\boldsymbol{y}\right)\, \boldsymbol{X}\left(\boldsymbol{X}^T\boldsymbol{X}\right)^{-1} \\ &= \left(\boldsymbol{X}^T\boldsymbol{X}\right)^{-1}\boldsymbol{X}^T\sigma^2\boldsymbol{I}_n\,\boldsymbol{X}\left(\boldsymbol{X}^T\boldsymbol{X}\right)^{-1} \\ &= \sigma^2\left(\boldsymbol{X}^T\boldsymbol{X}\right)^{-1}\boldsymbol{X}^T\boldsymbol{X}\left(\boldsymbol{X}^T\boldsymbol{X}\right)^{-1} \\ &= \sigma^2\left(\boldsymbol{X}^T\boldsymbol{X}\right)^{-1} \end{aligned}$$

Using this, the standard error (i.e. the estimated standard deviation) of $\hat{\beta}_j$ (for any j in $1, \ldots, p$) is

$$StdErr\left(\hat{\beta}_j\right) = \sqrt{\hat{\sigma}^2 \left[\left(\boldsymbol{X}^T\boldsymbol{X}\right)^{-1}\right]_{jj}}$$

2.1.5 Confidence intervals and hypothesis tests

We can now state the general method of creating confidence intervals and perform hypothesis tests for any element of $\boldsymbol{\beta}$.

The confidence interval formula is (as usual)

$$\hat{\beta}_j \pm t_{n-p}^{1-\alpha/2}\, StdErr\left(\hat{\beta}_j\right)$$

and a test statistic for testing $H_0 : \beta_j = 0$ versus $H_a : \beta_j \neq 0$ is

$$t_{n-p} = \frac{\hat{\beta}_j - 0}{StdErr\left(\hat{\beta}_j\right)}$$

2.1.6 Summary of pertinent results

- $\hat{\boldsymbol{\beta}} = \left(\boldsymbol{X}^T\boldsymbol{X}\right)^{-1}\boldsymbol{X}^T\boldsymbol{y}$ is the unbiased maximum-likelihood estimator of $\boldsymbol{\beta}$.
- The Central Limit Theorem applies to each element of $\boldsymbol{\beta}$. That is, as $n \to \infty$, the distribution of $\hat{\beta}_j \to N\left(\beta_j, \left[\sigma^2\left(\boldsymbol{X}^T\boldsymbol{X}\right)^{-1}\right]_{jj}\right)$.
- The error terms can be calculated via

$$\begin{aligned} \hat{\boldsymbol{y}} &= \boldsymbol{X}\hat{\boldsymbol{\beta}} \\ \hat{\boldsymbol{\epsilon}} &= \boldsymbol{y} - \hat{\boldsymbol{y}} \end{aligned}$$

- The estimate of σ^2 is

$$\hat{\sigma}^2 = \frac{1}{n-p}\,\hat{\boldsymbol{\epsilon}}^T\hat{\boldsymbol{\epsilon}}$$

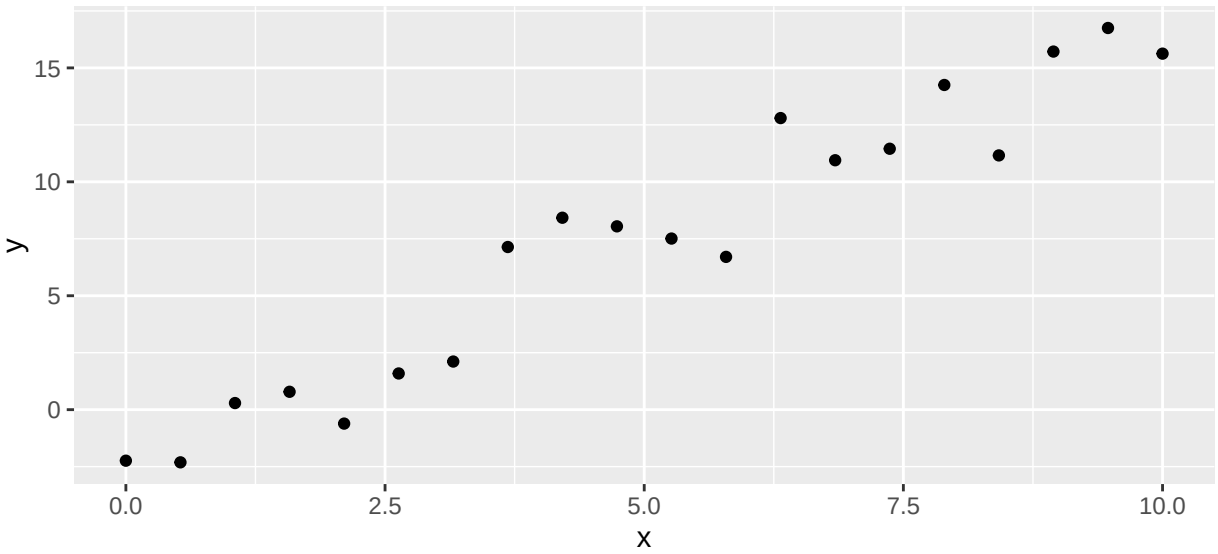
- The standard error (i.e. the estimated standard deviation) of $\hat{\beta}_j$ (for any j in $1, \ldots, p$) is

$$StdErr\left(\hat{\beta}_j\right) = \sqrt{\hat{\sigma}^2 \left[\left(\boldsymbol{X}^T\boldsymbol{X}\right)^{-1}\right]_{jj}}$$

2.1.7 An example in R

Here we will work an example in R and see the calculations. Consider the following data:

```
library(ggplot2)
n <- 20
x <- seq(0,10, length=n)
y <- -3 + 2*x + rnorm(n, sd=2)
my.data <- data.frame(x=x, y=y)
ggplot(my.data) + geom_point(aes(x=x,y=y))
```



First we must create the design matrix $\boldsymbol{X}$. Recall

$$\boldsymbol{X} = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ 1 & x_3 \\ \vdots & \vdots \\ 1 & x_{n-1} \\ 1 & x_n \end{bmatrix}$$

and can be created in R via the following:

```
X <- cbind( rep(1,n), x)
```

Given $\boldsymbol{X}$ and $\boldsymbol{y}$ we can calculate

$$\hat{\boldsymbol{\beta}} = \left(\boldsymbol{X}^T\boldsymbol{X}\right)^{-1}\boldsymbol{X}^T\boldsymbol{y}$$

in R using the following code:

```
XtXinv <- solve( t(X) %*% X )
beta.hat <- XtXinv %*% t(X) %*% y
beta.hat
```

```
##        [,1]
##   -2.454386
## x  1.952212
```

Our next step is to calculate the predicted values $\hat{\boldsymbol{y}}$ and the residuals $\hat{\boldsymbol{\epsilon}}$

$$\begin{aligned} \hat{\boldsymbol{y}} &= \boldsymbol{X}\hat{\boldsymbol{\beta}} \\ \hat{\boldsymbol{\epsilon}} &= \boldsymbol{y} - \hat{\boldsymbol{y}} \end{aligned}$$

```
y.hat <- X %*% beta.hat
residuals <- y - y.hat
```

Now that we have the residuals, we can calculate $\hat{\sigma}^2$ and the standard errors of $\hat{\beta}_j$

$$\hat{\sigma}^2 = \frac{1}{n-p}\,\hat{\boldsymbol{\epsilon}}^T\hat{\boldsymbol{\epsilon}}$$

$$StdErr\left(\hat{\beta}_j\right) = \sqrt{\hat{\sigma}^2 \left[\left(\boldsymbol{X}^T\boldsymbol{X}\right)^{-1}\right]_{jj}}$$

```
sigma2.hat <- ( t(residuals) %*% residuals) / (n-2)
sigma.hat <- sqrt( sigma2.hat )
std.errs <- sqrt(  diag(XtXinv) * sigma2.hat )
```

We now print out the important values and compare them to the summary output given by the `lm()` function in R.

```
beta.hat
```

```
##        [,1]
##   -2.454386
## x  1.952212
```

```
sigma.hat
```

```
##          [,1]
## [1,] 1.680327
```

```
std.errs
```

```
## [1] 0.7241298 0.1238045
```

```
model <- lm(y~x)
summary(model)
```

```
##
## Call:
## lm(formula = y ~ x)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -2.8258 -1.1816  0.1003  0.8468  2.9221
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)  -2.4544     0.7241  -3.389  0.00327 **
## x             1.9522     0.1238  15.769 5.57e-12 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 1.68 on 18 degrees of freedom
## Multiple R-squared:  0.9325, Adjusted R-squared:  0.9287
## F-statistic: 248.6 on 1 and 18 DF,  p-value: 5.571e-12
```

We calculate 95% confidence intervals via:

```
lwr <- beta.hat - qt(.975, n-2) * std.errs
upr <- beta.hat + qt(.975, n-2) * std.errs
CI <- cbind(lwr,upr)
colnames(CI) <- c('lower','upper')
rownames(CI) <- c('Intercept', 'x')
CI
```

```
##               lower      upper
## Intercept -3.975726 -0.9330458
## x          1.692108  2.2123156
```

These intervals are the same as what we get when we use the `confint()` function.

```
confint(model)
```

```
##                 2.5 %     97.5 %
## (Intercept) -3.975726 -0.9330458
## x            1.692108  2.2123156
```

2.2 ANOVA model

The anova model is also a linear model and all we must do is create a appropriate design matrix. Given the design matrix $\boldsymbol{X}$, all the calculations are identical as in the simple regression case.

2.2.1 Cell means representation

Recall the cell means representation is

$$y_{i,j} = \mu_i + \epsilon_{i,j}$$

where $y_{i,j}$ is the jth observation within the ith group. To clearly show the creation of the $\boldsymbol{X}$ matrix, let the number of groups be $p = 3$ and the number of observations per group be $n_i = 4$. We now expand the formula to show all the data.

$$\begin{aligned}
y_{1,1} &= \mu_1 + \epsilon_{1,1} \\
y_{1,2} &= \mu_1 + \epsilon_{1,2} \\
y_{1,3} &= \mu_1 + \epsilon_{1,3} \\
y_{1,4} &= \mu_1 + \epsilon_{1,4} \\
y_{2,1} &= \mu_2 + \epsilon_{2,1} \\
y_{2,2} &= \mu_2 + \epsilon_{2,2} \\
y_{2,3} &= \mu_2 + \epsilon_{2,3} \\
y_{2,4} &= \mu_2 + \epsilon_{2,4} \\
y_{3,1} &= \mu_3 + \epsilon_{3,1} \\
y_{3,2} &= \mu_3 + \epsilon_{3,2} \\
y_{3,3} &= \mu_3 + \epsilon_{3,3} \\
y_{3,4} &= \mu_3 + \epsilon_{3,4}
\end{aligned}$$

In an effort to write the model as $\boldsymbol{y} = \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$ we will write the above as

$$
\begin{aligned}
y_{1,1} &= 1\mu_1 + 0\mu_2 + 0\mu_3 + \epsilon_{1,1} \\
y_{1,2} &= 1\mu_1 + 0\mu_2 + 0\mu_3 + \epsilon_{1,2} \\
y_{1,3} &= 1\mu_1 + 0\mu_2 + 0\mu_3 + \epsilon_{1,3} \\
y_{1,4} &= 1\mu_1 + 0\mu_2 + 0\mu_3 + \epsilon_{1,4} \\
y_{2,1} &= 0\mu + 1\mu_2 + 0\mu_3 + \epsilon_{2,1} \\
y_{2,2} &= 0\mu + 1\mu_2 + 0\mu_3 + \epsilon_{2,2} \\
y_{2,3} &= 0\mu + 1\mu_2 + 0\mu_3 + \epsilon_{2,3} \\
y_{2,4} &= 0\mu + 1\mu_2 + 0\mu_3 + \epsilon_{2,4} \\
y_{3,1} &= 0\mu + 0\mu_2 + 1\mu_3 + \epsilon_{3,1} \\
y_{3,2} &= 0\mu + 0\mu_2 + 1\mu_3 + \epsilon_{3,2} \\
y_{3,3} &= 0\mu + 0\mu_2 + 1\mu_3 + \epsilon_{3,3} \\
y_{3,4} &= 0\mu + 0\mu_2 + 1\mu_3 + \epsilon_{3,4}
\end{aligned}
$$

and we will finally be able to write the matrix version

$$
\underbrace{\begin{bmatrix} y_{1,1} \\ y_{1,2} \\ y_{1,3} \\ y_{1,4} \\ y_{2,1} \\ y_{2,2} \\ y_{2,3} \\ y_{2,4} \\ y_{3,1} \\ y_{3,2} \\ y_{3,3} \\ y_{3,4} \end{bmatrix}}_{\boldsymbol{y}} = \underbrace{\begin{bmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \end{bmatrix}}_{\mathbf{X}} \underbrace{\begin{bmatrix} \mu_1 \\ \mu_2 \\ \mu_3 \end{bmatrix}}_{\boldsymbol{\beta}} + \underbrace{\begin{bmatrix} \epsilon_{1,1} \\ \epsilon_{1,2} \\ \epsilon_{1,3} \\ \epsilon_{1,4} \\ \epsilon_{2,1} \\ \epsilon_{2,2} \\ \epsilon_{2,3} \\ \epsilon_{2,4} \\ \epsilon_{3,1} \\ \epsilon_{3,2} \\ \epsilon_{3,3} \\ \epsilon_{3,4} \end{bmatrix}}_{\boldsymbol{\epsilon}}
$$

Notice that each column of the $\boldsymbol{X}$ matrix is acting as an indicator if the observation is an element of the appropriate group. As such, these are often called `indicator variables''. Another term for these, which I find less helpful, is`dummy variables".

2.2.2 Offset from reference group

In this model representation of ANOVA, we have an overall mean and then offsets from the control group (which will be group one). The model is thus

$$y_{i,j} = \mu + \tau_i + \epsilon_{i,j}$$

where $\tau_1 = 0$. We can write this in matrix form as

$$\underbrace{\begin{bmatrix} y_{1,1} \\ y_{1,2} \\ y_{1,3} \\ y_{1,4} \\ y_{2,1} \\ y_{2,2} \\ y_{2,3} \\ y_{2,4} \\ y_{3,1} \\ y_{3,2} \\ y_{3,3} \\ y_{3,4} \end{bmatrix}}_{\boldsymbol{y}} = \underbrace{\begin{bmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \\ 1 & 1 & 0 \\ 1 & 1 & 0 \\ 1 & 1 & 0 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \end{bmatrix}}_{\mathbf{X}} \underbrace{\begin{bmatrix} \mu \\ \tau_2 \\ \tau_3 \end{bmatrix}}_{\boldsymbol{\beta}} + \underbrace{\begin{bmatrix} \epsilon_{1,1} \\ \epsilon_{1,2} \\ \epsilon_{1,3} \\ \epsilon_{1,4} \\ \epsilon_{2,1} \\ \epsilon_{2,2} \\ \epsilon_{2,3} \\ \epsilon_{2,4} \\ \epsilon_{3,1} \\ \epsilon_{3,2} \\ \epsilon_{3,3} \\ \epsilon_{3,4} \end{bmatrix}}_{\boldsymbol{\epsilon}}$$

2.3 Exercises

1. We will do a simple ANOVA analysis on example 8.2 from Ott & Longnecker using the matrix representation of the model. A clinical psychologist wished to compare three methods for reducing hostility levels in university students, and used a certain test (HLT) to measure the degree of hostility. A high score on the test indicated great hostility. The psychologist used 24 students who obtained high and nearly equal scores in the experiment. eight were selected at random from among the 24 problem cases and were treated with method 1. Seven of the remaining 16 students were selected at random and treated with method 2. The remaining nine students were treated with method 3. All treatments were continued for a one-semester period. Each student was given the HLT test at the end of the semester, with the results show in the following table. (This analysis was done in section 8.3 of my STA 570 notes)

Method	Values
1	96, 79, 91, 85, 83, 91, 82, 87
2	77, 76, 74, 73, 78, 71, 80
3	66, 73, 69, 66, 77, 73, 71, 70, 74

We will be using the cell means model of ANOVA

$$y_{ij} = \beta_i + \epsilon_{ij}$$

where β_i is the mean of group i and $\epsilon_{ij} \overset{iid}{\sim} N\left(0, \sigma^2\right)$.

a. Create one vector of all 24 hostility test scores `y`. (Use the `c()` function.)

b. Create a design matrix `X` with dummy variables for columns that code for what group an observation belongs to. Notice that `X` will be a 24 rows by 3 column matrix. An R function that might be handy is `cbind(a,b)` which will bind two vectors or matrices together along the columns. (There is also a corresponding `rbind()` function that binds vectors/matrices along rows.)

c) Find $\hat{\boldsymbol{\beta}}$ using the matrix formula given in class. The R function `t(A)` computes the matrix transpose $\mathbf{A}^T$, `solve(A)` computes $\mathbf{A}^{-1}$, and the operator `%*%` does matrix multiplication (used as `A %*% B`).

d) Examine the matrix $\left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T$. What do you notice about it? In particular, think about the result when you right multiply by $\mathbf{y}$. How does this matrix calculate the appropriate group means and using the appropriate group sizes n_i?

2. We will calculate the y-intercept and slope estimates in a simple linear model using matrix notation. We will use a data set that gives the diameter at breast height (DBH) versus tree height for a randomly selected set of trees. In addition, for each tree, a ground measurement of crown closure (CC) was taken. Larger values of crown closure indicate more shading and is often associated with taller tree morphology (possibly). We will be interested in creating a regression model that predicts height based on DBH and CC. In the interest of reduced copying, we will only use 10 observations. *(Note: I made this data up and the DBH values might be unrealistic. Don't make fun of me.)*

DBH	30.5	31.5	31.7	32.3	33.3	35	35.4	35.6	36.3	37.8
CC	0.74	0.69	0.65	0.72	0.58	0.5	0.6	0.7	0.52	0.6
Height	58	64	65	70	68	63	78	80	74	76

We are interested in fitting the regression model

$$y_i = \beta_0 + \beta_1 x_{i,1} + \beta_2 x_{i,2} + \epsilon_i$$

where β_0 is the y-intercept and β_1 is the slope parameter associated with DBH and β_2 is the slope parameter associated with Crown Closure.

a) Create a vector of all 10 heights $\mathbf{y}$.
b) Create the design matrix $\mathbf{X}$.
c) Find $\hat{\boldsymbol{\beta}}$ using the matrix formula given in class.
d) Compare your results to the estimated coefficients you get using the `lm()` function. To add the second predictor to the model, your call to `lm()` should look something like `lm(Height ~ DBH + CrownClosure)`.

Chapter 3

Inference

3.1 F-tests

We wish to develop a rigorous way to compare nested models and decide if a complicated model explains enough more variability than a simple model to justify the additional intellectual effort of thinking about the data in the complicated fashion.

It is important to specify that we are developing a way of testing nested models. By nested, we mean that the simple model can be created from the full model just by setting one or more model parameters to zero.

3.1.1 Theory

Recall that in the simple regression and ANOVA cases we were interested in comparing a simple model versus a more complex model. For each model we computed the residual sum of squares (RSS) and said that if the complicated model performed much better than the simple then $RSS_{simple} \gg RSS_{complex}$. To do this we needed to standardize by the number of parameters added to the model and the degrees of freedom remaining in the full model. We first defined $RSS_{diff} = RSS_{simple} - RSS_{complex}$ and let df_{diff} be the number of parameters difference between the simple and complex models. Then we had

$$F = \frac{RSS_{difference}/df_{diff}}{RSS_{complex}/df_{complex}}$$

and we claimed that if the null hypothesis was true (i.e. the complex model is an unnecessary obfuscation of the simple), then this ratio follows an F -distribution with degrees of freedom df_{diff} and $df_{complex}$.

The critical assumption for the F-test to be appropriate is that the error terms are independent and normally distributed with constant variance.

We will consider a data set from Johnson and Raven (1973) which also appears in Weisberg (1985). This data set is concerned with the number of tortoise species on $n = 30$ different islands in the Galapagos. The variables of interest in the data set are:

Variable	Description
`Species`	Number of tortoise species found on the island
`Endimics`	Number of tortoise species endemic to the island
`Elevation`	Elevation of the highest point on the island
`Area`	Area of the island (km^2)
`Nearest`	Distance to the nearest neighboring island (km)
`Scruz`	Distance to the Santa Cruz islands (km)
`Adjacent`	Area of the nearest adjacent island (km^2)

We will first read in the data set from the package `faraway`.

```
library(faraway)    # load the library
data(gala)          # import the data set
head(gala)          # show the first couple of rows
```

```
##              Species Endemics  Area Elevation Nearest Scruz Adjacent
## Baltra            58       23 25.09       346     0.6   0.6     1.84
## Bartolome         31       21  1.24       109     0.6  26.3   572.33
## Caldwell           3        3  0.21       114     2.8  58.7     0.78
## Champion          25        9  0.10        46     1.9  47.4     0.18
## Coamano            2        1  0.05        77     1.9   1.9   903.82
## Daphne.Major      18       11  0.34       119     8.0   8.0     1.84
```

First we will create the full model that predicts the number of species as a function of elevation, area, nearest, scruz and adjacent. Notice that this model has $p = 6$ β_i values (one for each coefficient plus the intercept).

```
M.c <- lm(Species ~ Area + Elevation + Nearest + Scruz + Adjacent, data=gala)
summary(M.c)
```

```
##
## Call:
## lm(formula = Species ~ Area + Elevation + Nearest + Scruz + Adjacent,
##     data = gala)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -111.679  -34.898   -7.862   33.460  182.584
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)  7.068221  19.154198   0.369 0.715351
## Area        -0.023938   0.022422  -1.068 0.296318
## Elevation    0.319465   0.053663   5.953 3.82e-06 ***
## Nearest      0.009144   1.054136   0.009 0.993151
## Scruz       -0.240524   0.215402  -1.117 0.275208
## Adjacent    -0.074805   0.017700  -4.226 0.000297 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 60.98 on 24 degrees of freedom
## Multiple R-squared:  0.7658, Adjusted R-squared:  0.7171
## F-statistic:  15.7 on 5 and 24 DF,  p-value: 6.838e-07
```

3.1.2 Testing All Covariates

The first test we might want to do is to test if any of the covariates are significant. That is to say that we want to test the full model versus the simple null hypothesis model

$$y_i = \beta_0 + \epsilon_i$$

that has no covariates and only a y-intercept. So we will create a simple model

```
M.s <- lm(Species ~ 1, data=gala)
```

and calculate the appropriate Residual Sums of Squares (RSS) for each model, along with the difference in degrees of freedom between the two models.

```
RSS.c <- sum(resid(M.c)^2)
RSS.s <- sum(resid(M.s)^2)
df.diff <- 5               # complex model has 5 additional parameters
df.c <- 30 - 6             # complex model has 24 degrees of freedom left
```

The F-statistic for this test is therefore

```
F.stat <-  ( (RSS.s - RSS.c) / df.diff ) / ( RSS.c / df.c )
F.stat
```

```
## [1] 15.69941
```

and should be compared against the F-distribution with 5 and 24 degrees of freedom. Because a large difference between RSS.s and RSS.c would be evidence for the alternative, larger model, the p-value for this test is

$$p - value = P\left(F_{5,24} \geq \texttt{F.stat}\right)$$

```
p.value <-  1 - pf(15.699, 5, 24)
p.value
```

```
## [1] 6.839486e-07
```

Both the F.stat and its p-value are given at the bottom of the summary table. However, I might be interested in creating an ANOVA table for this situation.

Source	df	Sum Sq	Mean Sq	F	p-value
Difference	$p-1$	RSS_d	$MSE_d = RSS_d/(p-1)$	MSE_d/MSE_c	$P(F > F_{p-1,n-p})$
Complex	$n-p$	RSS_c	$MSE_c = RSS_c/(n-p)$		
Simple	$n-1$	RSS_s			

This table can be obtained from R by using the `anova()` function on the two models of interest. As usual with R, it does not show the simple row, but rather concentrates on the difference row.

```
anova(M.s, M.c)
```

```
## Analysis of Variance Table
##
## Model 1: Species ~ 1
## Model 2: Species ~ Area + Elevation + Nearest + Scruz + Adjacent
##   Res.Df    RSS Df Sum of Sq      F    Pr(>F)
## 1     29 381081
## 2     24  89231  5    291850 15.699 6.838e-07 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

3.1.3 Testing a Single Covariate

For a particular covariate, β_j, we might wish to perform a test to see if it can be removed from the model. It can be shown that the F-statistic can be re-written as

$$
\begin{aligned}
F &= \frac{\left[RSS_s - RSS_c\right]/1}{RSS_c/\left(n-p\right)} \\
&= \vdots \\
&= \left[\frac{\hat{\beta}_j}{SE\left(\hat{\beta}_j\right)}\right]^2 \\
&= t^2
\end{aligned}
$$

where t has a t-distribution with $n-p$ degrees of freedom under the null hypothesis that the simple model is sufficient.

We consider the case of removing the covariate `Area` from the model and will calculate our test statistic using both methods.

```
M.c <- lm(Species ~ Area + Elevation + Nearest + Scruz + Adjacent, data=gala)
M.s <- lm(Species ~        Elevation + Nearest + Scruz + Adjacent, data=gala)
RSS.c <- sum( resid(M.c)^2 )
RSS.s <- sum( resid(M.s)^2 )
df.d <- 1
df.c <- 30-6
F.stat <- ((RSS.s - RSS.c)/1) / (RSS.c / df.c)
F.stat
```

```
## [1] 1.139792
```

```
1 - pf(F.stat, 1, 24)
```

```
## [1] 0.296318
```

```
sqrt(F.stat)
```

```
## [1] 1.067611
```

To calculate it using the estimated coefficient and its standard error, we must grab those values from the summary table

```
temp <- summary(M.c)
temp$coefficients
```

```
##                 Estimate  Std. Error      t value     Pr(>|t|)
## (Intercept)  7.068220709 19.15419782  0.369016796 7.153508e-01
## Area        -0.023938338  0.02242235 -1.067610554 2.963180e-01
## Elevation    0.319464761  0.05366280  5.953187968 3.823409e-06
## Nearest      0.009143961  1.05413595  0.008674366 9.931506e-01
## Scruz       -0.240524230  0.21540225 -1.116628222 2.752082e-01
## Adjacent    -0.074804832  0.01770019 -4.226216850 2.970655e-04
```

```
beta.area <- temp$coefficients[2,1]
SE.beta.area <- temp$coefficients[2,2]
t <- beta.area / SE.beta.area
t
```

```
## [1] -1.067611
```

```
2 * pt(t, 24)
```

```
## [1] 0.296318
```

All that hand calculation is tedious, so we can again use the anova() command to compare the two models.

```
anova(M.s, M.c)
```

```
## Analysis of Variance Table
##
## Model 1: Species ~ Elevation + Nearest + Scruz + Adjacent
## Model 2: Species ~ Area + Elevation + Nearest + Scruz + Adjacent
##   Res.Df   RSS Df Sum of Sq      F Pr(>F)
## 1     25 93469
## 2     24 89231  1    4237.7 1.1398 0.2963
```

3.1.4 Testing a Subset of Covariates

Often a researcher will want to remove a subset of covariates from the model. In the Galapagos example, Area, Nearest, and Scruz all have non-significant p-values and would be removed when comparing the full model to the model without that one covariate. While each of them might be non-significant, is the sum of all three significant?

Because the individual $\hat{\beta}_j$ values are not independent, then we cannot claim that the subset is not statistically significant just because each variable in turn was insignificant. Instead we again create simple and complex models in the same fashion as we have previously done.

```
M.c <- lm(Species ~ Area + Elevation + Nearest + Scruz + Adjacent, data=gala)
M.s <- lm(Species ~        Elevation +                   Adjacent, data=gala)
anova(M.s, M.c)
```

```
## Analysis of Variance Table
##
## Model 1: Species ~ Elevation + Adjacent
## Model 2: Species ~ Area + Elevation + Nearest + Scruz + Adjacent
##   Res.Df    RSS Df Sum of Sq      F Pr(>F)
## 1     27 100003
## 2     24  89231  3     10772 0.9657  0.425
```

We find a large p-value associated with this test and can safely stay with the null hypothesis, that the simple model is sufficient to explain the observed variability in the number of species of tortoise.

3.2 Confidence Intervals for location parameters

Recall that

$$\hat{\boldsymbol{\beta}} \sim N\left(\boldsymbol{\beta}, \sigma^2 \left(\mathbf{X}^T\mathbf{X}\right)^{-1}\right)$$

and it is easy to calculate the estimate of σ^2. This estimate will be the "average" squared residual

$$\hat{\sigma}^2 = \frac{RSS}{df}$$

where RSS is the residual sum of squares and df is the degrees of freedom $n - p$ where p is the number of β_j parameters. Therefore the standard error of the $\hat{\beta}_j$ values is

$$SE\left(\hat{\beta}_j\right) = \sqrt{\hat{\sigma}^2 \left(\mathbf{X}^T\mathbf{X}\right)^{-1}_{jj}}$$

We can see this calculation in the summary regression table. We again consider the Galapagos Island data set. First we must create the design matrix

```
y <- gala$Species
X <- cbind( rep(1,30), gala$Elevation, gala$Adjacent )
```

And then create $\left(\mathbf{X}^T\mathbf{X}\right)^{-1}$

```
XtXinv <- solve(  t(X) %*% X )
XtXinv
```

```
##               [,1]          [,2]          [,3]
## [1,]  6.094829e-02 -8.164025e-05  9.312123e-06
## [2,] -8.164025e-05  2.723835e-07 -7.126027e-08
## [3,]  9.312123e-06 -7.126027e-08  6.478031e-08
```

```
diag(XtXinv)
```

```
## [1] 6.094829e-02 2.723835e-07 6.478031e-08
```

Eventually we will need $\hat{\boldsymbol{\beta}}$

```
beta.hat <- XtXinv %*% t(X) %*% y
beta.hat
```

```
##            [,1]
## [1,]  1.4328722
## [2,]  0.2765683
## [3,] -0.0688855
```

And now find the estimate $\hat{\sigma}$

```
H <- X %*% XtXinv %*% t(X)
y.hat <- H %*% y
RSS <- sum( (y-y.hat)^2 )
sigma.hat <- sqrt(  RSS/(30-3) )
sigma.hat
```

```
## [1] 60.85898
```

The standard errors of $\hat{\beta}$ is thus

```
sqrt( sigma.hat^2 * diag(XtXinv) )
```

```
## [1] 15.02468680  0.03176253  0.01548981
```

We can double check that this is what R calculates in the summary table

```
model <- lm(Species ~ Elevation + Adjacent, data=gala)
summary(model)
```

```
##
## Call:
## lm(formula = Species ~ Elevation + Adjacent, data = gala)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -103.41  -34.33  -11.43   22.57  203.65
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)  1.43287   15.02469   0.095 0.924727
## Elevation    0.27657    0.03176   8.707 2.53e-09 ***
## Adjacent    -0.06889    0.01549  -4.447 0.000134 ***
```

```
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 60.86 on 27 degrees of freedom
## Multiple R-squared:  0.7376, Adjusted R-squared:  0.7181
## F-statistic: 37.94 on 2 and 27 DF,  p-value: 1.434e-08
```

It is highly desirable to calculate confidence intervals for the regression parameters. Recall that the general form of a confidence interval is

$$Estimate \pm Critical\,Value \cdot StandardError\,(Estimate)$$

For any specific β_j we will have

$$\hat{\beta}_j \pm t_{n-p}^{1-\alpha/2}\,\hat{\sigma}\sqrt{(\mathbf{X}^T\mathbf{X})_{jj}^{-1}}$$

where $\hat{\sigma}^2\left(\mathbf{X}^T\mathbf{X}\right)_{jj}^{-1}$ is the $[j,j]$ element of the variance/covariance of $\hat{\boldsymbol{\beta}}$.

To demonstrate this, we return to the Galapagos Island data set.

Finally we can calculate confidence intervals for our three β_j values

```
lower <- beta.hat - qt(.975, 27) * sigma.hat * sqrt( diag(XtXinv) )
upper <- beta.hat + qt(.975, 27) * sigma.hat * sqrt( diag(XtXinv) )
cbind(lower, upper)
```

```
##             [,1]        [,2]
## [1,] -29.395239 32.26098305
## [2,]   0.211397  0.34173962
## [3,]  -0.100668 -0.03710303
```

That is certainly a lot of work to do by hand (even with R doing all the matrix multiplication) but we can get these from R by using the confint() command.

```
confint(model)
```

```
##                   2.5 %      97.5 %
## (Intercept) -29.395239 32.26098305
## Elevation     0.211397  0.34173962
## Adjacent     -0.100668 -0.03710303
```

3.3 Prediction and Confidence Intervals for a response

Given a vector of predictor covariates $\boldsymbol{x}_0$ (think of $\boldsymbol{x}_0^T$ as potentially one row in $\boldsymbol{X}$. Because we might want to predict some other values than what we observe, we do not restrict ourselves to *only* rows in $\boldsymbol{X}$), we want to make inference on the expected value $\hat{y}_0$. We can calculate the value by

$$\hat{y}_0 = \boldsymbol{x}_0^T\hat{\boldsymbol{\beta}}$$

and we are interested in two different types of predictions.

1. We might be interested in the uncertainty of a new data point. This uncertainty has two components: the uncertainty of the regression model and uncertainty of a new data point from its expected value.
2. Second, we might be interested in only the uncertainty about the regression model.

We note that because $\boldsymbol{x}_0^T$ is just a constant, we can calculate the variance of this value as

$$\begin{aligned} Var\left(\boldsymbol{x}_0^T\hat{\boldsymbol{\beta}}\right) &= \boldsymbol{x}_0^T\, Var\left(\hat{\boldsymbol{\beta}}\right)\, \boldsymbol{x}_0 \\ &= \boldsymbol{x}_0^T \left(\boldsymbol{X}^T\boldsymbol{X}\right)^{-1} \sigma^2\, \boldsymbol{x}_0 \\ &= \boldsymbol{x}_0^T \left(\boldsymbol{X}^T\boldsymbol{X}\right)^{-1} \boldsymbol{x}_0\, \sigma^2 \end{aligned}$$

and use this to calculate two types of intervals. First, a prediction interval for a new observation is

$$\hat{y}_0 \pm t_{n-p}^{1-\alpha/2}\, \hat{\sigma} \sqrt{1 + \boldsymbol{x}_0^T \left(\boldsymbol{X}^T\boldsymbol{X}\right)^{-1} \boldsymbol{x}_0}$$

and a confidence interval for the mean response for the given $\boldsymbol{x}_0$ is

$$\hat{y}_0 \pm t_{n-p}^{1-\alpha/2}\, \hat{\sigma} \sqrt{\boldsymbol{x}_0^T \left(\boldsymbol{X}^T\boldsymbol{X}\right)^{-1} \boldsymbol{x}_0}$$

Again using the Galapagos Island data set as an example, we might be interested in predicting the number of tortoise species of an island with highest point 400 meters and nearest adjacent island with area $200 km^2$. We then have

$$\boldsymbol{x}_0^T = \begin{bmatrix} 1 & 400 & 200 \end{bmatrix}$$

and we can calculate

```
x0 <- c(1, 400, 200)
y0 <- t(x0) %*% beta.hat
y0
```

```
##           [,1]
## [1,] 98.28309
```

and then calculate $\boldsymbol{x}_0^T \left(\boldsymbol{X}^T\boldsymbol{X}\right)^{-1} \boldsymbol{x}_0$

```
xt.XtXinv.x <- t(x0) %*% solve( t(X) %*% X ) %*% x0
```

Thus the prediction interval will be

```
c(y0 - qt(.975, 27) * sigma.hat * sqrt(1 + xt.XtXinv.x),
  y0 + qt(.975, 27) * sigma.hat * sqrt(1 + xt.XtXinv.x))
```

```
## [1] -28.70241 225.26858
```

while a confidence interval for the expectation is

```
c(y0 - qt(.975, 27) * sigma.hat * sqrt(xt.XtXinv.x),
  y0 + qt(.975, 27) * sigma.hat * sqrt(xt.XtXinv.x))
```

```
## [1]  75.21317 121.35301
```

These prediction and confidence intervals can be calculated in R using the predict() function

```
x0 <- data.frame(Elevation=400, Adjacent=200)
predict(model, newdata=x0, interval='prediction')
```

```
##        fit       lwr      upr
## 1 98.28309 -28.70241 225.2686
```

```
predict(model, newdata=x0, interval='confidence')
```

```
##        fit      lwr     upr
## 1 98.28309 75.21317 121.353
```

3.4 Interpretation with Correlated Covariates

The standard interpretation of the slope parameter is that β_j is the amount of increase in y for a one unit increase in the jth covariate, provided that all other covariates stayed the same.

The difficulty with this interpretation is that covariates are often related, and the phrase "all other covariates stayed the same" is often not reasonable. For example, if we have a dataset that models the mean annual temperature of a location as a function of latitude, longitude, and elevation, then it is not physically possible to hold latitude, and longitude constant while changing elevation.

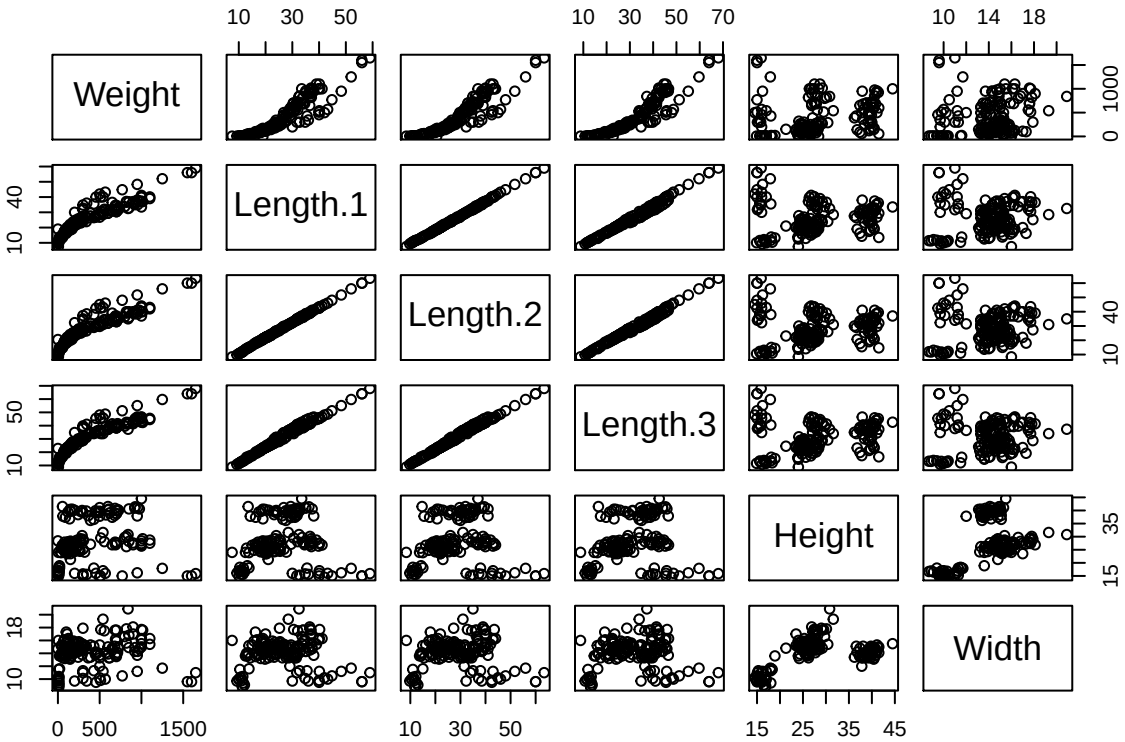
One common issue that make interpretation difficult is that covariates can be highly correlated.

Perch Example: We might be interested in estimating the weight of a fish based off of its length and width. The dataset we will consider is from fishes are caught from the same lake (Laengelmavesi) near Tampere in Finland. The following variables were observed:

Variable	Interpretation
`Weight`	Weight (g)
`Length.1`	Length from nose to beginning of Tail (cm)
`Length.2`	Length from nose to notch of Tail (cm)
`Length.3`	Length from nose to tip of tail (cm)
`Height`	Maximal height as a percentage of `Length.3`
`Width`	Maximal width as a percentage of `Length.3`
`Sex`	0=Female, 1=Male
`Species`	Which species of perch (1-7)

We first look at the data and observe the expected relationship between length and weight.

```
file <- 'https://raw.githubusercontent.com/dereksonderegger/STA_571_Book/master/data-raw/Fish.csv'
fish <- read.table(file, header=TRUE, skip=111, sep=',')
pairs(fish[,c('Weight','Length.1','Length.2','Length.3','Height','Width')])
```



Naively, we might consider the linear model with all the length effects present.

```
model <- lm(Weight ~ Length.1 + Length.2 + Length.3 + Height + Width, data=fish)
summary(model)
```

```
##
## Call:
## lm(formula = Weight ~ Length.1 + Length.2 + Length.3 + Height +
##     Width, data = fish)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -302.22  -79.72  -39.88   92.63  344.85
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept) -724.539     77.133  -9.393   <2e-16 ***
## Length.1      32.389     45.134   0.718   0.4741
## Length.2      -9.184     48.367  -0.190   0.8497
## Length.3       8.747     16.283   0.537   0.5919
## Height         4.947      2.768   1.787   0.0759 .
## Width          8.636      6.972   1.239   0.2174
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 132.9 on 152 degrees of freedom
##   (1 observation deleted due to missingness)
## Multiple R-squared:  0.8675, Adjusted R-squared:  0.8631
## F-statistic:   199 on 5 and 152 DF,  p-value: < 2.2e-16
```

This is crazy. There is a negative relationship between `Length.2` and `Weight`. That does not make any sense unless you realize that this is the effect of `Length.2` assuming the other covariates are in the model and can be held constant while changing the value of `Length.2`, which is obviously ridiculous.

If we remove the highly correlated covariates then we see a much better behaved model

```
model <- lm(Weight ~ Length.2 + Height + Width, data=fish)
summary(model)
```

```
##
## Call:
## lm(formula = Weight ~ Length.2 + Height + Width, data = fish)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -306.14  -75.11  -36.45   89.54  337.95
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept) -701.0750    71.0438  -9.868  < 2e-16 ***
## Length.2      30.4360     0.9841  30.926  < 2e-16 ***
## Height         5.5141     1.4311   3.853 0.000171 ***
## Width          5.6513     5.2016   1.086 0.278974
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 132.3 on 154 degrees of freedom
```

```
##   (1 observation deleted due to missingness)
## Multiple R-squared:  0.8669, Adjusted R-squared:  0.8643
## F-statistic: 334.2 on 3 and 154 DF,  p-value: < 2.2e-16
```

When you have two variables in a model that are highly positively correlated, you often find that one will have a positive coefficient and the other will be negative. Likewise, if two variables are highly negatively correlated, the two regression coefficients will often be the same sign.

In this case the sum of the three length covariate estimates was approximately 31 in both cases, but with three length variables, the second could be negative the third be positive with approximately the same magnitude and we get approximately the same model as with both the second and third length variables missing from the model.

In general, you should be very careful with the interpretation of the regression coefficients when the covariates are highly correlated. We will talk about how to recognize these situations and what to do about them later in the course.

3.5 Exercises

1. The dataset prostate in package `faraway` has information about a study of 97 men with prostate cancer. We import the data and examine the first four observations using the following commands.

   ```
   library(faraway)
   data(prostate)
   head(prostate)
   ```

   It is possible to get information about the data set using the command `help(prostate)`. Fit a model with `lpsa` as the response and all the other variables as predictors.

   a) Compute 90% and 95% confidence intervals for the parameter associated with `age`. Using just these intervals, what could we deduced about the p-value for age in the regression summary. *Hint: look at the help for the function* `confint()`. *You'll find the* `level` *option to be helpful.*

   b) Remove all the predictors that are not significant at the 5% level. Test this model against the original model. Which is preferred?

2. Thirty samples of cheddar cheese were analyzed for their content of acetic acid, hydrogen sulfide and lactic acid. Each sample was tasted and scored by a panel of judges and the average taste score produces. Used the `cheddar` dataset from the `faraway` package (import it the same way you did in problem one, but now use `cheddar`) to answer the following:

   a) Fit a regression model with taste as the response and the three chemical contents as predictors. Identify the predictors that are statistically significant at the 5% level.

   b) `Acetic` and `H2S` are measured on a $\log_{10}$ scale. Create two new columns in the `cheddar` data frame that contain the values on their original scale. Fit a linear model that uses the three covariates on their non-log scale. Identify the predictors that are statistically significant at the 5% level for this model.

   c) Can we use an F-test to compare these two models? Explain why or why not. Which model provides a better fit to the data? Explain your reasoning.

   d) If H2S is increased by 0.01 for the model in (a), what change in taste would be expected? What caveates must be made in this interpretation.

3. The `sat` data set in the `faraway` package gives data collected to study the relationship between expenditures on public education and test results.

   a) Fit a model that with `total` SAT score as the response and only the intercept as a covariate.

b) Fit a model with `total` SAT score as the response and `expend`, `ratio`, and `salary` as predictors (along with the intercept).

c) Compare the models in parts (a) and (b) using an F-test. Is the larger model superior?

d) Examine the summary table of the larger model? Does this contradict your results in part (c)? What might be causing this issue? Create a graph or summary diagnostics to support your guess.

e) Fit the model with `salary` and `ratio` (along with the intercept) as predictor variables and examine the summary table. Which covariates are significant?

f) Now add `takers` to the model (so the model now includes three predictor variables along with the intercept). Test the hypothesis that $\beta_{takers} = 0$ using the summary table. Compare this model to the previous one using an F-test. Demonstrate that the F-test and t-test are equivalent by noting the mathematical relationship between the t and F statistics and the equality of the p-values.

Bibliography