

# **Biological Statistics II**

**BTRY3020/STSCI3200 - Spring 2024**

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# Chapter 1: Vectors & Matrices

## Section 1: Basics

### Definition:

An  $r \times c$  **matrix**  $X$  is an  $r \times c$  array of values where  $r$  is the number of rows and  $c$  is the number of columns. The element in the  $i^{th}$  row and  $j^{th}$  column is denoted by  $x_{i,j}$ .<sup>1</sup>

$$X = \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1c} \\ x_{21} & x_{22} & \cdots & x_{2c} \\ \vdots & \vdots & & \vdots \\ x_{r1} & x_{r2} & \cdots & x_{rc} \end{bmatrix}$$

```
# Matrix X
X <- matrix(6:1, nrow = 2, ncol = 3, byrow = TRUE)
X
      [,1] [,2] [,3]
[1,]    6    5    4
[2,]    3    2    1
X[2, 3]
[1] 1
```

### Definition:

The **dimension** of a matrix is the ordered pair  $(r, c)$ .

```
dim(X)
[1] 2 3
```

## Section 2: Special Matrices

### Definition:

A **column vector** is an  $r \times 1$  matrix.<sup>2</sup>

$$X = \begin{bmatrix} x_{11} \\ x_{21} \\ \vdots \\ x_{i1} \\ \vdots \\ x_{r1} \end{bmatrix} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_i \\ \vdots \\ x_r \end{bmatrix}$$

### Definition:

A **row vector** is a  $1 \times c$  matrix.<sup>3</sup>

$$X = [x_{11} \quad x_{12} \quad \cdots \quad x_{1j} \quad \cdots \quad x_{1c}] = [x_1 \quad x_2 \quad \cdots \quad x_j \quad \cdots \quad x_c]$$

<sup>1</sup> When it will not cause confusion, the comma is left out.

<sup>2</sup> When it will not cause confusion, only the row index will be listed.

<sup>3</sup> When it will not cause confusion, only the column index will be listed.

**Definition:**

A **square** matrix is an  $r \times c$  matrix where  $r = c$ .

```
# Matrix Z
Z <- matrix(c(-1, 0, 5, 7, 10, -1, 9, 5, 2), nrow = 3, ncol = 3, byrow = TRUE)
Z
      [,1] [,2] [,3]
[1,]   -1    0    5
[2,]    7   10   -1
[3,]    9    5    2
dim(Z)
[1] 3 3
```

**Definition:**

The **transpose** of an  $r \times c$  matrix  $X = [x_{ij}]$  is an  $c \times r$  matrix  $X^T = [(X^T)_{ij} = x_{ji}]$ .

$$X^T = \begin{bmatrix} x_{11} & x_{21} & \cdots & x_{c1} \\ x_{12} & x_{22} & \cdots & x_{c2} \\ \vdots & \vdots & x_{ji} & \vdots \\ x_{1r} & x_{2r} & \cdots & x_{cr} \end{bmatrix}$$

```
#### Original Matrix
```

```
X
      [,1] [,2] [,3]
[1,]    6    5    4
[2,]    3    2    1
```

```
#### Result
```

```
t(X)
      [,1] [,2]
[1,]    6    3
[2,]    5    2
[3,]    4    1
```

**Definition:**

Suppose  $X$  is a square matrix. If  $X = X^T$  then  $X$  is called **symmetric**.

**Definition:**

A **diagonal** matrix  $X$  is a matrix where the elements  $x_{ij} = 0$  whenever  $i \neq j$ . The elements on the **main diagonal** of  $X$  are those elements  $x_{ii}$  where  $i = j$ .

```
D <- diag(c(5, 7, 9), nrow = 3, ncol = 5)
D
      [,1] [,2] [,3] [,4] [,5]
[1,]    5    0    0    0    0
[2,]    0    7    0    0    0
[3,]    0    0    9    0    0
```

**Definition:**

An  $n \times n$  **identity** matrix  $I_n$  is a square diagonal matrix with ones on the main diagonal.

```
I <- diag(3)
I
      [,1] [,2] [,3]
[1,]    1    0    0
[2,]    0    1    0
[3,]    0    0    1
```

### Section 3: Operations

#### Scalar Multiplication:

The **scalar multiple** of a  $r \times c$  matrix  $X = [x_{ij}]$  by constant  $k$  is given by  $kX = [(kX)_{ij} = kx_{ij}]$

```
#### Original Matrix
X
      [,1] [,2] [,3]
[1,]    6    5    4
[2,]    3    2    1
#### Scalar
k <- 3

#### Result
Y <- k * X
Y
      [,1] [,2] [,3]
[1,]   18   15   12
[2,]    9    6    3
```

#### Matrix Addition:

The sum of two  $r \times c$  matrices  $X = [x_{ij}]$  and  $Y = [y_{ij}]$  is given by  $X + Y = [(X + Y)_{ij} = x_{ij} + y_{ij}]$ <sup>4</sup>

```
#### Original Matrices
X
      [,1] [,2] [,3]
[1,]    6    5    4
[2,]    3    2    1

Y
      [,1] [,2] [,3]
[1,]   18   15   12
[2,]    9    6    3

#### Result
X + Y
      [,1] [,2] [,3]
[1,]   24   20   16
[2,]   12    8    4
```

#### Inner Product:

The **inner product** of two  $n \times 1$  column vectors  $X$  and  $Y$  is given by

$$\langle X, Y \rangle = x_1y_1 + x_2y_2 + \cdots + x_ny_n.$$

$$\langle X, Y \rangle = \left\langle \begin{bmatrix} 1 \\ 2 \\ 3 \\ 4 \end{bmatrix}, \begin{bmatrix} 5 \\ 6 \\ 7 \\ 8 \end{bmatrix} \right\rangle = (1 \times 5) + (2 \times 6) + (3 \times 7) + (4 \times 8).$$

<sup>4</sup> Matrices can not be added if they do not have the same dimensions. A row and column vector can not be added together. Remember, a vector is  $R$  is not the same thing as a row/column vector.

## Matrix Multiplication

### Matrix Multiplication of a row and column vector:

The product  $XY$  of a  $1 \times n$  row matrix  $X$  (on the left) and an  $n \times 1$  column matrix  $Y$  (on the right) is given by

$$XY = x_1y_1 + x_2y_2 + \cdots + x_ny_n$$

$$(= \langle X^T, Y \rangle).$$

$$XY = \begin{bmatrix} 1 & 2 & 3 & 4 \end{bmatrix} \begin{bmatrix} 5 \\ 6 \\ 7 \\ 8 \end{bmatrix} = (1 \times 5) + (2 \times 6) + (3 \times 7) + (4 \times 8)$$

### General Matrix Multiplication:

The product of an  $r \times d$  matrix  $X = [x_{ij}]$  and a  $d \times c$  matrix  $Y = [y_{ij}]$  is given by an  $r \times c$  matrix  $XY = [(XY)_{ij} = X_i \cdot Y_j]$ .

$$\begin{bmatrix} \leftarrow & X_1. & \rightarrow \\ \leftarrow & X_2. & \rightarrow \\ \vdots & \vdots & \vdots \\ \leftarrow & X_r. & \rightarrow \end{bmatrix} \begin{bmatrix} \uparrow & \uparrow & \cdots & \uparrow \\ Y_{.1} & Y_{.2} & \cdots & Y_{.c} \\ \downarrow & \downarrow & \cdots & \downarrow \end{bmatrix} = \begin{bmatrix} X_1.Y_1 & X_1.Y_2 & \cdots & X_1.Y_c \\ X_2.Y_1 & X_2.Y_2 & \cdots & X_2.Y_c \\ \vdots & \vdots & X_i.Y_j & \vdots \\ X_r.Y_1 & X_r.Y_2 & \cdots & X_r.Y_c \end{bmatrix}$$

### Example:

Determine the dimension of each of the following products:

$$XY = \begin{bmatrix} 6 & 5 & 4 \\ 3 & 2 & 1 \end{bmatrix} \begin{bmatrix} -1 & 2 \\ -3 & 4 \\ -5 & 6 \end{bmatrix} \qquad YX = \begin{bmatrix} -1 & 2 \\ -3 & 4 \\ -5 & 6 \end{bmatrix} \begin{bmatrix} 6 & 5 & 4 \\ 3 & 2 & 1 \end{bmatrix}$$

### Example:

Determine the dimension of each of the following products and compute the entries:

a.  $XZ = \begin{bmatrix} 6 & 5 & 4 \\ 3 & 2 & 1 \end{bmatrix} \begin{bmatrix} -1 & 0 & 5 \\ 7 & 10 & -1 \\ 9 & 5 & 2 \end{bmatrix}$

```
X %%% Z
      [,1] [,2] [,3]
[1,]   65   70   33
[2,]   20   25   15
```

b.  $ZX = \begin{bmatrix} -1 & 0 & 5 \\ 7 & 10 & -1 \\ 9 & 5 & 2 \end{bmatrix} \begin{bmatrix} 6 & 5 & 4 \\ 3 & 2 & 1 \end{bmatrix}$

```
Z %%% X
Error in Z %%% X: non-conformable arguments
```



### Facts about Matrix Multiplication

1. Suppose  $X$  is an  $r \times t$  matrix and  $Y$  is a  $v \times c$  matrix.
  - a. The product  $XY$  is only defined when  $t = v$ .
  - b. If  $t \neq v$ , the matrices are said to be **non-conformable**.
2. Matrix Multiplication is **not** commutative.
  - a.  $XY$  may not equal  $YX$
3. Matrix Multiplication is distributive
  - a.  $X(Y + Z) = XY + XZ$
  - b.  $(Y + Z)X = YX + ZX$
4. Matrix Multiplication is associative
  - a.  $(XY)Z = X(YZ)$
5.  $(XY)^T = Y^T X^T$

## Section 4: Inverses

### Recall:

An  $n \times n$  **identity** matrix  $I_n$  is a square diagonal matrix with ones on the main diagonal.

### Definition:

The **inverse** of a matrix  $X$ , if such a matrix exists, denoted by  $X^{-1}$  is any matrix such that  $X(X^{-1}) = (X^{-1})X = I$ . A matrix with an inverse is called **invertible**. Otherwise, it is called **singular**.

```
mat <- matrix(c(1, 2, 4, 1), nrow = 2)
mat
      [,1] [,2]
[1,]    1    4
[2,]    2    1

matInv <- solve(mat)
matInv
      [,1] [,2]
[1,] -0.1428571  0.5714286
[2,]  0.2857143 -0.1428571

mat %*% matInv
      [,1] [,2]
[1,]    1    0
[2,]    0    1
```

1. Suppose  $X$  is an  $r \times c$ , then
  - a.  $I_r X = X$
  - b.  $X I_c = X$
2. If a matrix is invertible then it is a square matrix.
  - a. A square matrix can be singular.
3. If a matrix is singular then one row(column) is a sum of multiples of the other rows(columns).
4. If  $X$  is symmetric and invertible, then  $(X^T)^{-1} = X^{-1}$

## Section 5: Random Matrices

### Definition:

A **random matrix**  $X$  is an  $r \times c$  matrix whose elements are random variables  $X_{ij}$ .

$$X = \begin{bmatrix} X_{11} & X_{12} & \cdots & X_{1c} \\ X_{21} & X_{22} & \cdots & X_{2c} \\ \vdots & \vdots & X_{ij} & \vdots \\ X_{r1} & X_{r2} & \cdots & X_{rc} \end{bmatrix}.$$

### Definition:

A **random column vector** is an  $r \times 1$  random matrix. A **random row vector** is an  $1 \times c$  random matrix<sup>5</sup>.

### Expected Value

The **mean**, or **expected value**  $(\mu_X, E(X))$ , of a random variable  $X$  is

$$E(X) = \mu = \begin{cases} \sum_{x \in S} x p(x) & X \text{ is discrete} \\ \int_{-\infty}^{\infty} x f(x) dx & X \text{ is continuous.} \end{cases}$$

### Definition:

The **expected value**  $E(X)$  of a  $r \times c$  random matrix  $X$  is given by

$$E(X) = \begin{bmatrix} E(X_{11}) & E(X_{12}) & \cdots & E(X_{1c}) \\ E(X_{21}) & E(X_{22}) & \cdots & E(X_{2c}) \\ \vdots & \vdots & E(X_{ij}) & \vdots \\ E(X_{r1}) & E(X_{r2}) & \cdots & E(X_{rc}) \end{bmatrix}.$$

### Facts:

1. A random sample  $X_1, X_2, \dots, X_n$  can be represented with a random column vector  $X = [X_1 \ X_2 \ \cdots \ X_n]^T$ .
2. Matrix operations can be carried out between random and non-random matrices.
3. If  $A$  a matrix of constants,  $X$  is a random vector,  $b$  is a constant vector, and  $Y = AX + b$ , then  $E(Y) = AE(X) + b$ .

### Example:

Suppose  $X$  is a random vector with  $n \geq 1$  independent and identically distributed elements, and  $1_n$  is an  $n$  element row vector whose elements are all ones. Determine  $E\left(\frac{1}{n}1_n X\right)$ .

<sup>5</sup> First, unless it will cause confusion, when a random column/row vector is being used, only one indexing value will be used. Second, assume a given vector is a column vector if there is no indication given as to whether it is a row or column vector.

## Covariance

### Definition:

The **covariance** of a two random variables  $X, Y$  is  $Cov(X, Y) = E[(X - \mu_X)(Y - \mu_Y)]$ .

$$Cov(X, Y) = \begin{cases} \sum_{(x,y) \in S} (x - \mu_X)(y - \mu_Y)p(x, y) & (X, Y) \text{ is discrete} \\ \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} (x - \mu_X)(y - \mu_Y)f(x, y) dx dy & f(x, y) \text{ is continuous.} \end{cases}$$

The **variance** of a random variable  $X$  is  $Cov(X, X)$ .

$$V(X) = \begin{cases} \sum_{x \in S} (x - \mu)^2 p(x) & X \text{ is discrete} \\ \int_{-\infty}^{\infty} (x - \mu)^2 f(x) dx & X \text{ is continuous.} \end{cases}$$

### Definition:

The **variance/covariance matrix**  $V(X)$  of a  $n$  element random vector  $X$  with mean vector  $\mu = E(X) = [\mu_1 \ \mu_2 \ \cdots \ \mu_n]^T$  is given by

$$V(X) = E[(X - \mu)(X - \mu)^T]$$

$$\begin{aligned} &= E \left( \begin{bmatrix} X_1 - \mu_1 \\ X_2 - \mu_2 \\ \vdots \\ X_n - \mu_n \end{bmatrix} [X_1 - \mu_1 \ X_2 - \mu_2 \ \cdots \ X_n - \mu_n] \right) \\ &= E \begin{bmatrix} (X_1 - \mu_1)^2 & (X_1 - \mu_1)(X_2 - \mu_2) & \cdots & (X_1 - \mu_1)(X_n - \mu_n) \\ (X_2 - \mu_2)(X_1 - \mu_1) & (X_2 - \mu_2)^2 & \cdots & (X_2 - \mu_2)(X_n - \mu_n) \\ \vdots & \vdots & \ddots & \vdots \\ (X_n - \mu_n)(X_1 - \mu_1) & (X_n - \mu_n)(X_2 - \mu_2) & \cdots & (X_n - \mu_n)^2 \end{bmatrix} \end{aligned}$$

### Facts:

Suppose  $X$  is a random vector with  $n$  elements.

1.  $V(X)$  is an  $n \times n$ (square) symmetric matrix.
  - a. The values on the main diagonal represent the variances of each element of  $X$ .
  - b. The values off the main diagonal represent covariances.
2. If the elements of  $X$  are independent, then  $V(X)$  is a diagonal matrix.
3. If  $A$  a matrix of constants,  $b$  is a constant vector,  $Y = AX + b$ , and the matrix operations make sense, then  $V(Y) = AV(X)A^T$ .

### Example:

Suppose  $X$  is a random vector with  $n \geq 1$  independent and identically distributed elements, and  $1_n$  is an  $n$  element row vector whose elements are all ones. Determine  $V\left(\frac{1}{n}1_n X\right)$ .



## Chapter 2: Regression Analysis

### Definition:

**Regression Analysis** is a statistical methodology that examines the relationship between a (collection of) predictor variable(s)  $X$  and a response variable  $Y$ . The goal is to predict a value for the response based on a specified values of the predictor(s).

In some situations,

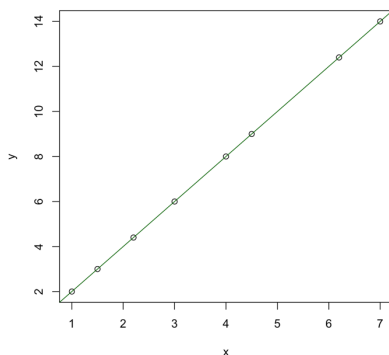
- predictor variables could be referred to as independent or explanatory variables;
- response variables could be referred to as dependent or outcome variables.

### Section 1: Relations between Variables

#### Functional Relationship:

The response variable  $Y$  is a function  $f(X)$  of the predictor variable(s)  $X$ .

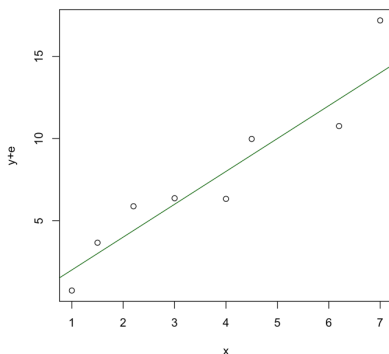
```
set.seed(1)
par(mfrow = c(1, 1))
x <- c(1, 3, 4, 7, 1.5, 6.2, 4.5, 2.2)
ln <- length(x)
y <- 2 * x
plot(x, y)
abline(0, 2, col = "darkgreen")
```



#### Statistical Relationship:

The response variable  $Y$  is not a function of the predictor variable(s)  $X$ . However, given a value of  $X$ , something is known about  $Y$ .<sup>6</sup>

```
y.plus.e <- y + rnorm(ln, sd = 2)
plot(x, y.plus.e, ylab = "y+e")
abline(0, 2, col = "darkgreen")
```



<sup>6</sup> In some cases, there is no interesting relationship between the predictor(s) and the response.

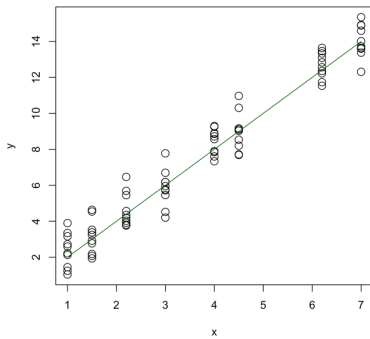
## Section 2: Regression Models

### Definition:

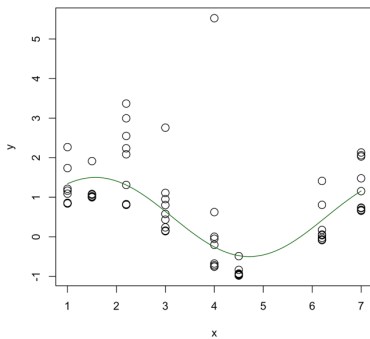
A **regression model** is a formal description of the statistical relationship. The model specifies two characteristics:

1. The probability distribution of the response variable at each level of the predictor variables.
2. The functional relationship between the mean of the response variable and the predictor variables.

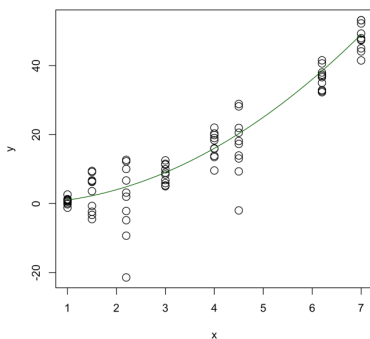
```
set.seed(4)
x <- rep(c(1, 3, 4, 7, 1.5, 6.2, 4.5, 2.2), times = 10)
ln <- length(x)
y <- 2 * x + rnorm(ln)
plot(x, y, cex = 1.5)
curve(2 * x, from = 1, to = 7, col = "darkgreen", add = T)
```



```
y <- sin(x) + rchisq(ln, df = 0.5)
plot(x, y, cex = 1.5)
curve(sin(x) + 0.5, from = 1, to = 7, col = "darkgreen", add = T)
```



```
y <- x^2 + rnorm(ln, sd = 1:(ln/10))
plot(x, y, cex = 1.5)
curve(x^2, from = 1, to = 7, col = "darkgreen", add = T)
```



### Section 3: Simple Linear Regression - Unspecified Error

#### Simple Linear Regression Model:

A **simple linear regression** model relates the response variable  $Y_i$  and a single predictor variable  $X_i$  as follows:

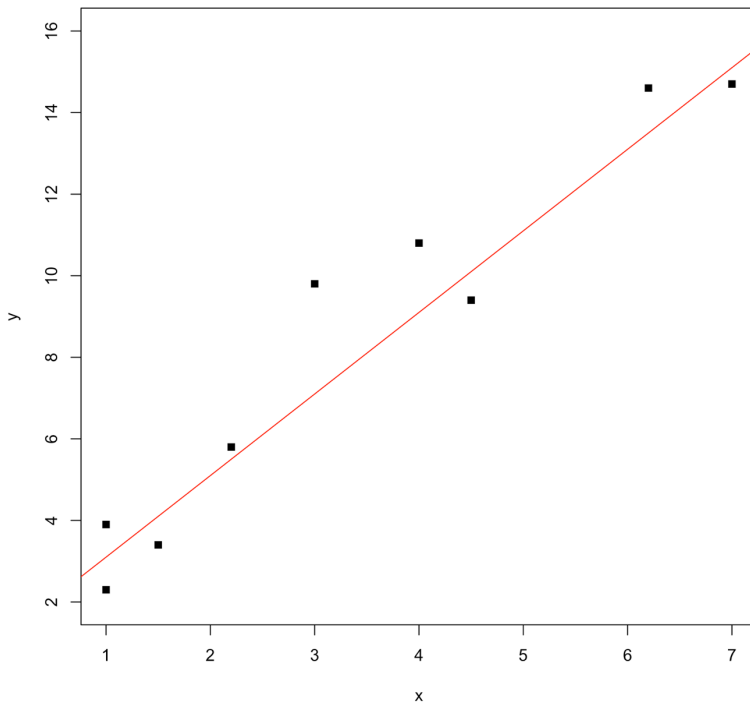
$$Y_i = \beta_0 + \beta_1 X_i + \epsilon_i$$

where

1.  $Y_i$  is the value of the response in the  $i^{th}$  trial.
2.  $\beta_0, \beta_1$  are unknown intercept and slope parameters.
3.  $X_i$  is the value of the predictor in the  $i^{th}$  trial, and is a known constant.
4.  $\epsilon_i$  is the random error (variable) on the  $i^{th}$  trial where  $E(\epsilon_i) = 0$ ,  $V(\epsilon_i) = \sigma^2 > 0$ , and  $Cov(\epsilon_i, \epsilon_j) = 0$  for all  $i \neq j$

$$Y = \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{bmatrix} \quad X = \begin{bmatrix} 1 & X_1 \\ 1 & X_2 \\ \vdots & \vdots \\ 1 & X_n \end{bmatrix} \quad \beta = \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} \quad \epsilon = \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{bmatrix}$$

(1,2.3) (3,9.8) (4,10.8) (7,14.7) (1.5,3.4) (6.2,14.6) (4.5,9.4) (2.2,5.8) (1,3.9)



```
set.seed(14)
x <- c(1, 3, 4, 7, 1.5, 6.2, 4.5, 2.2, 1)
error <- rchisq(9, df = 1) - 1
y <- 2 * x + 1.1 + error
y <- round(y, digits = 1)
plot(x, y, pch = 15, ylim = c(2, 16))
abline(a = 1.1, b = 2, col = "red")
```

## Section 4: Estimation of Regression Function

### Method of Least Squares

#### Definition:

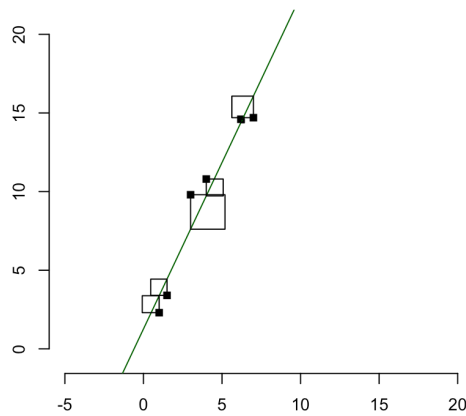
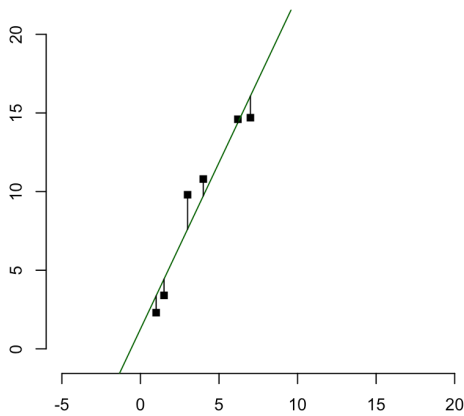
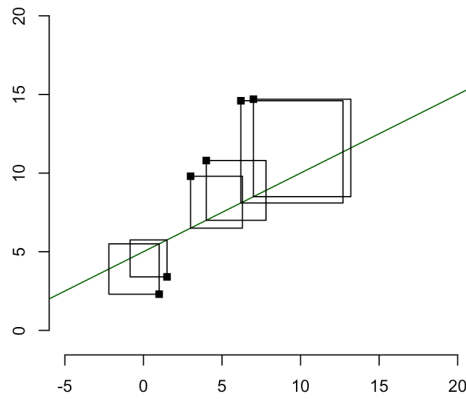
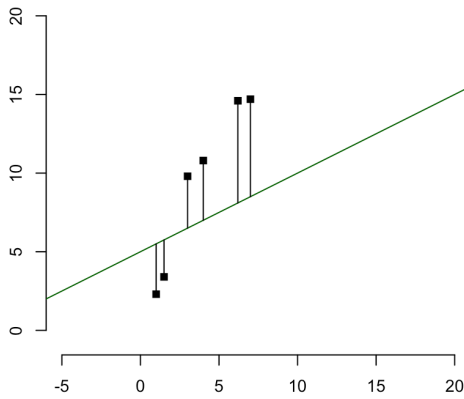
Given a data set  $(X_1, Y_1), (X_2, Y_2), \dots, (X_n, Y_n)$ , the **method of least squares** estimates the intercept  $\beta_0$  and slope  $\beta_1$  parameters. It works by minimizing the function

$$\begin{aligned} SS(b_0^*, b_1^*) &= \sum_{i=1}^n [y_i - (b_0^* + b_1^* X_i)]^2 \\ &= (Y - Xb^*)^T (Y - Xb^*) \end{aligned}$$

The values of  $b_0^*$  and  $b_1^*$  that minimize  $SS(b_0^*, b_1^*)$  will be denoted by  $b_0$  and  $b_1$ .

- $b_0$  will be called the **least squares estimate** of the intercept  $\beta_0$ .
- $b_1$  will be called the **least squares estimate** of the slope  $\beta_1$ .

$$SS(b_0, b_1) \leq \min_{\substack{\text{all intercepts } b_0^* \\ \text{all slopes } b_1^*}} SS(b_0^*, b_1^*)$$





**Least Squares Estimators**

$$b = \begin{bmatrix} b_0 \\ b_1 \end{bmatrix}$$

$$\beta = \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix}$$

1. For the simple linear regression model, the least squares estimates of  $\beta_0$  and  $\beta_1$  are given by

$$b_0 = \bar{y} - \bar{x}b_1 \qquad b_1 = \frac{\sum_{i=1}^n (X_i - \bar{X})(Y_i - \bar{Y})}{\sum_{i=1}^n (X_i - \bar{X})^2}$$

2. Different methods exist for minimizing  $SS(b_0^*, b_1^*)$ .

a. Guess and Check

b. Calculus

c. Matrix Algebra

3. For the simple linear regression model,  $b_0$  and  $b_1$  are the solutions to the **normal equations**.

$$\begin{aligned} \sum Y_i &= nb_0 + b_1 \sum X_i \\ \sum X_i Y_i &= b_0 \sum X_i + b_1 \sum X_i^2 \end{aligned} \qquad X^T Y = X^T X b$$

4. For the simple linear regression model, the least squares estimates  $b_0$  and  $b_1$  are unbiased estimates of  $\beta_0$  and  $\beta_1$ .

5. For the simple linear regression model, the least squares estimates  $b_0$  and  $b_1$  have the smallest variance among all possible unbiased linear estimates of  $\beta_0$  and  $\beta_1$ .

### Point Estimate of the Mean Response

#### **Definition:**

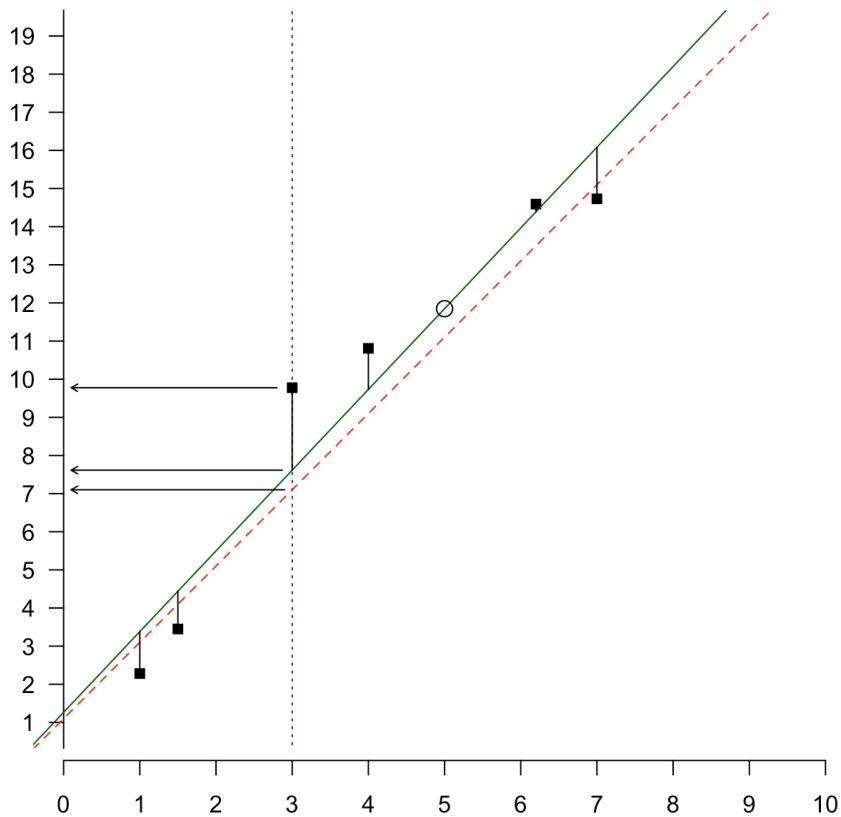
The **equation of the least squares regression line** is given by

$$\hat{Y} = b_0 + b_1X,$$

where  $b_0$  and  $b_1$  are estimates of  $\beta_0$  and  $\beta_1$ .

#### **Definition:**

The **mean response** at  $X$  is given by  $E(Y) = \beta_0 + \beta_1X$ . The estimate of the mean response at  $X$  is given by evaluating the equation of the least squares regression line at  $X$ . When  $X$  is one of the observed values of the independent variable, the **mean response** at  $X$  is called a **fitted value**.



### Residuals

#### **Definition:**

The  $i^{th}$  **residual**  $e_i$  is the difference between the  $i^{th}$  observed value and the  $i^{th}$  fitted value. That is,

$$e = \begin{bmatrix} e_1 \\ e_2 \\ \vdots \\ e_n \end{bmatrix} = \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{bmatrix} - \begin{bmatrix} \hat{Y}_1 \\ \hat{Y}_2 \\ \vdots \\ \hat{Y}_n \end{bmatrix}$$

**Definition:**

The  $i^{th}$  **residual**  $e_i$  is the difference between the  $i^{th}$  observed value and the  $i^{th}$  fitted value. That is,

$$e_i = Y_i - \hat{Y}_i.$$

**Properties of the Fitted Regression Line**

1. The sum of the residuals is zero.  $\sum e_i = 0$
  
2. The sum of the squared residuals is a minimum.
  
3. The sum of the observed values is equal to the sum of the fitted values:  $\sum Y_i = \sum \hat{Y}_i$ .
  
4. The sum of the weighted residuals is zero, when the weight on the  $i^{th}$  residual is  $X_i$ :  $\sum X_i e_i = 0$ .
  
5. The sum of the weighted residuals is zero, when the weight on the  $i^{th}$  residual is  $\hat{Y}_i$ :  $\sum \hat{Y}_i e_i = 0$ .
  
6. The regression line always goes through the point  $(\bar{X}, \bar{Y})$ :  $\bar{Y} = b_0 + b_1 \bar{X}$

## Section 5: Estimating the Variance of the Error

$$\sigma^2 = E[(Y - \mu_Y)^2]$$

### Single Population

#### Known Mean

$$s^2 = \frac{\sum_{i=1}^n (Y_i - \mu_Y)^2}{n}$$

#### Unknown Mean

$$SSE = \sum (Y_i - \bar{Y})^2$$

$$DFE = n - 1$$

$$s^2 = \frac{SSE}{DFE}$$

#### Regression $\sigma^2 = V(\epsilon) = V(Y | X)$

The **sum of square error (SSE)** or **sum of square residuals (SSR)** is given by  $SSE = \sum (Y_i - \hat{Y}_i)^2$ .

The **degrees of freedom error (DFE)**<sup>7</sup> or **degrees of freedom residuals (DFR)** is given by  $DFE = n - 2$ .

$$SSE = \sum (Y_i - \hat{Y}_i)^2$$

$$DFE = n - 2$$

$$s^2 = \frac{SSE}{DFE}$$

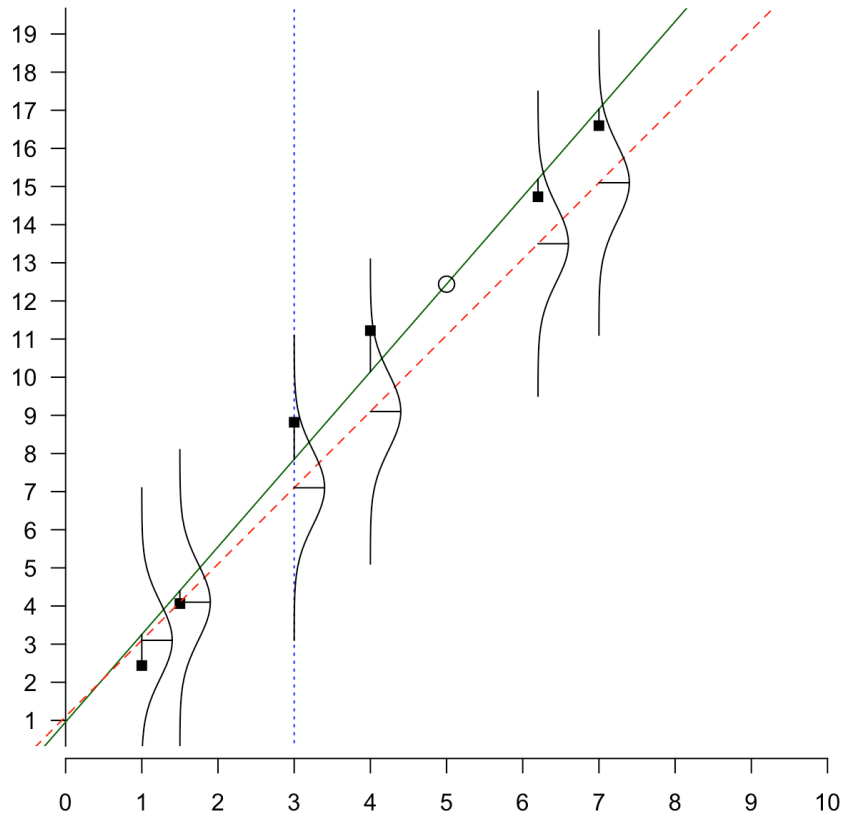
---

<sup>7</sup> In many cases, the degrees of freedom can be computed using the following guide: DF = number of independent pieces of information (n) minus number of estimated parameters.

## Section 6: Normal Errors

### Normal Error Regression Model:

A **normal error regression** model is a simple linear regression model where the  $\epsilon_i$  are independent normally distributed random variables with mean zero and common variance  $\sigma^2$ .



### Maximum Likelihood Estimators

When the distribution of the error terms are specified, another method can be used to estimate  $\beta_0$ ,  $\beta_1$ , and  $\sigma^2$ .

#### **Definition:**

Given a random variable  $X$  with density function  $f(x|\theta)$ , that is dependent on a parameter  $\theta$ , and an observed value of  $X = x$ , the **likelihood function** is  $L(\theta|x) = f(x|\theta)$ .

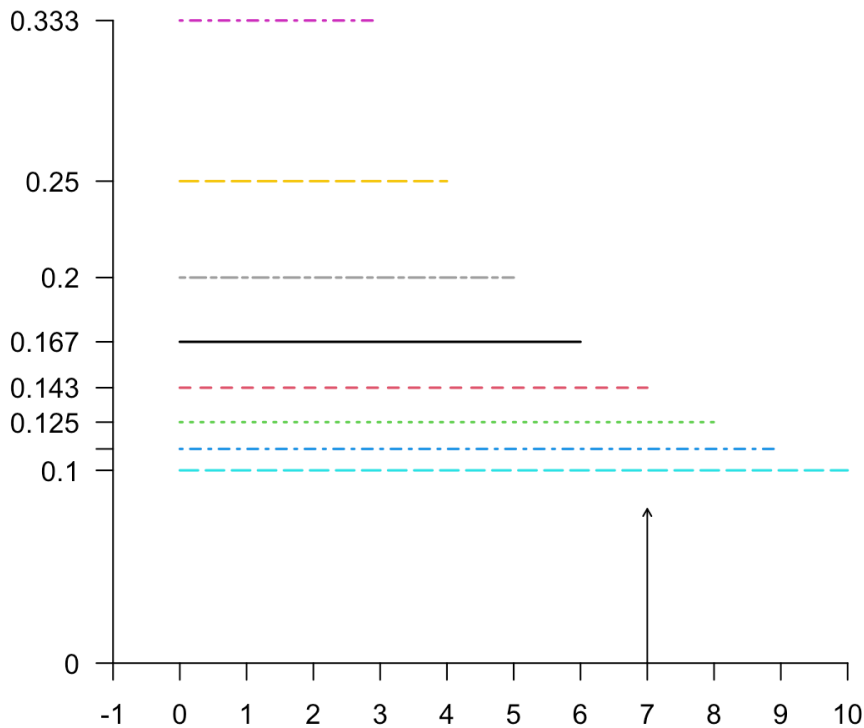
#### **Definition:**

The **maximum likelihood estimate** of a parameter  $\theta$  is the value (mle  $\theta$ ) that makes the observed data most likely.

$$L(\text{mle } \theta|x) = \max_{\text{all possible } \theta} L(\theta|x)$$

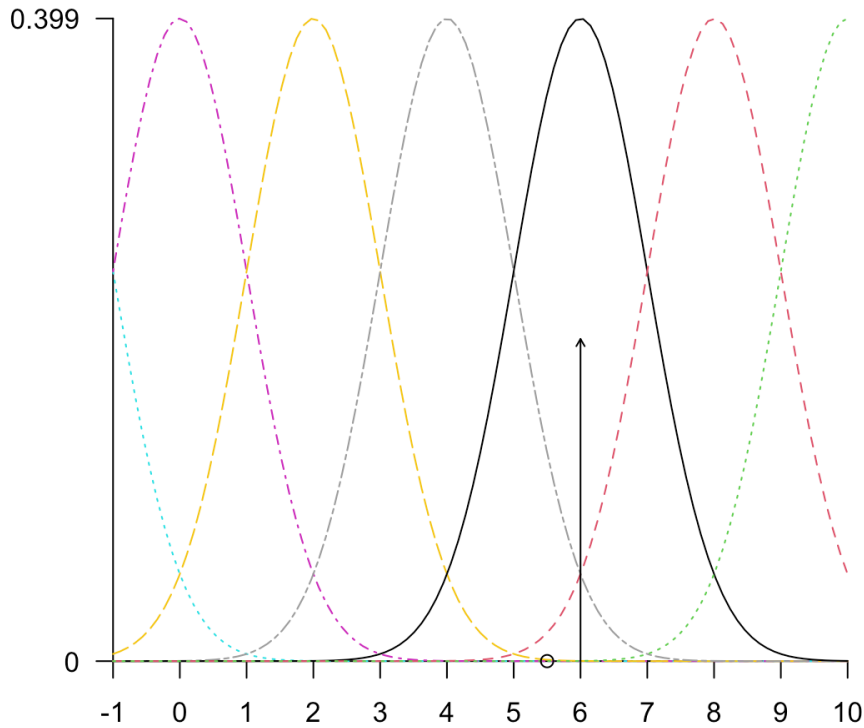
#### **Example:**

Suppose a population follows a uniform distribution on the interval  $[0, b]$ . You have taken a sample of size 1. The observed value is 7. Determine the maximum likelihood estimate of  $b$ .



**Example:**

Suppose a population follows a normal distribution with a standard deviation of one. You have taken a sample of size 1. The observed value is 5.5. Determine the maximum likelihood estimate of the mean of the distribution.

**Properties of Maximum Likelihood Estimators**

1. If  $\hat{\theta}$  is a maximum likelihood estimator of a parameter  $\theta$ , and  $g(\theta)$  is a function of  $\theta$ , then  $g(\hat{\theta})$  is a maximum likelihood estimator of a parameter  $g(\theta)$ .
2. Using the normal regression model, the maximum likelihood estimators of  $\beta_0$  and  $\beta_1$  are  $b_0$  and  $b_1$ , respectively.
3. Using the normal regression model, the maximum likelihood estimators of  $\sigma^2$  is  $\frac{\sum (y_i - \hat{y}_i)^2}{n}$ .

## Section 7: Example & Code

### Example:

The director of admissions at a college wants to describe the GPA of a freshmen at the end of their freshmen year based upon their ACT score. They will fit a simple linear model.

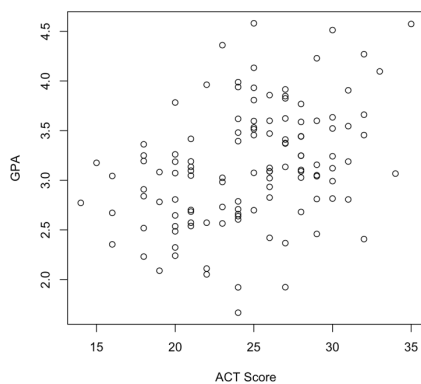
*#### A portion of the dataset*

```
head(SLRSet1)
  GPA ACT
1 2.539076 21
2 2.772057 14
3 2.680529 28
4 3.962266 22
5 3.134735 21
6 2.806456 31
```

*#### Sample Size*

```
nrow(SLRSet1)
[1] 120
```

```
plot(SLRSet1$ACT, SLRSet1$GPA, xlab = "ACT Score", ylab = "GPA")
```



*#### Fitting Linear Model*

```
lm.fit <- lm(GPA ~ ACT, data = SLRSet1)
```

*#### Output of Fitted Model*

```
lm.fit
```

Call:

```
lm(formula = GPA ~ ACT, data = SLRSet1)
```

Coefficients:

```
(Intercept)      ACT
  1.89783      0.05034
```

*#### Summarized Output of Fitted Model*

```
summary(lm.fit)
```

Call:

```
lm(formula = GPA ~ ACT, data = SLRSet1)
```

Residuals:

```
      Min       1Q   Median       3Q      Max
-1.44000 -0.37148 -0.04281  0.36769  1.42492
```

Coefficients:

```
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  1.89783    0.28280   6.711 7.11e-10 ***
ACT          0.05034    0.01126   4.472 1.80e-05 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```
Residual standard error: 0.5492 on 118 degrees of freedom
Multiple R-squared:  0.1449,    Adjusted R-squared:  0.1377
F-statistic:    20 on 1 and 118 DF,  p-value: 1.796e-05
```



#### #### Contents of Fitted Model

```
names(lm.fit)
[1] "coefficients" "residuals"      "effects"      "rank"
[5] "fitted.values" "assign"          "qr"           "df.residual"
[9] "xlevels"      "call"           "terms"        "model"
```

```
coefficients(lm.fit)
(Intercept)      ACT
1.89783001  0.05033694
```

#### #### Computing Fitted Values

```
predict(lm.fit)[1:5]
      1      2      3      4      5
2.954906 2.602547 3.307264 3.005243 2.954906
```

```
fitted.values(lm.fit)[1:5]
      1      2      3      4      5
2.954906 2.602547 3.307264 3.005243 2.954906
```

#### #### Computing Estimates of Mean Response

```
coefficients(lm.fit)[1] + coefficients(lm.fit)[2] * c(4, 0, 2.1)
[1] 2.099178 1.897830 2.003538
```

```
nd <- data.frame(ACT = c(4, 0, 2.1))
predict(lm.fit, newdata = nd)
      1      2      3
2.099178 1.897830 2.003538
```

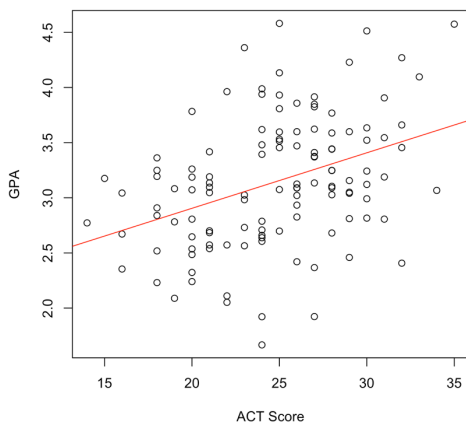
#### #### Computing residual

```
SLRSet1$GPA[1:5] - fitted.values(lm.fit)[1:5]
      1      2      3      4      5
-0.4158302 0.1695100 -0.6267357 0.9570229 0.1798295
```

```
residuals(lm.fit)[1:5]
      1      2      3      4      5
-0.4158302 0.1695100 -0.6267357 0.9570229 0.1798295
sd(residuals(lm.fit))
[1] 0.5468474
```

#### #### Alternative Graphing Method

```
plot(GPA ~ ACT, data = SLRSet1, xlab = "ACT Score", ylab = "GPA")
abline(coefficients(lm.fit), col = "red")
```





## Chapter 3: Inference with Simple Linear Regression

### Data

$$(X_1, Y_1), (X_2, Y_2), \dots, (X_i, Y_i), \dots, (X_n, Y_n)$$

### Linear Model

$$\begin{array}{rclclcl} Y_1 & = & \beta_0 \cdot 1 & + & \beta_1 X_1 & + & \epsilon_1 \\ Y_2 & = & \beta_0 \cdot 1 & + & \beta_1 X_2 & + & \epsilon_2 \\ \vdots & & \vdots & & \vdots & & \vdots \\ Y_i & = & \beta_0 \cdot 1 & + & \beta_1 X_i & + & \epsilon_i \\ \vdots & & \vdots & & \vdots & & \vdots \\ Y_n & = & \beta_0 \cdot 1 & + & \beta_1 X_n & + & \epsilon_n \end{array}$$

$$\begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_i \\ \vdots \\ Y_n \end{bmatrix} = \beta_0 \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \\ \vdots \\ 1 \end{bmatrix} + \beta_1 \begin{bmatrix} X_1 \\ X_2 \\ \vdots \\ X_i \\ \vdots \\ X_n \end{bmatrix} + \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_i \\ \vdots \\ \epsilon_n \end{bmatrix}$$

$$\begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_i \\ \vdots \\ Y_n \end{bmatrix} = \begin{bmatrix} 1 & X_1 \\ 1 & X_2 \\ \vdots & \vdots \\ 1 & X_i \\ \vdots & \vdots \\ 1 & X_n \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} + \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_i \\ \vdots \\ \epsilon_n \end{bmatrix}$$

### Parameter Estimates

#### Slope & Intercept:

$$b = \begin{bmatrix} b_0 \\ b_1 \end{bmatrix} = \begin{bmatrix} \bar{Y} - b_1 \bar{X} \\ \frac{\sum (X_i - \bar{X})(Y_i - \bar{Y})}{\sum (X_i - \bar{X})^2} \end{bmatrix} = (X^T X)^{-1} X^T Y$$

$$E(b) = \begin{bmatrix} E(b_0) \\ E(b_1) \end{bmatrix} = \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix}$$

#### Standard Errors:

$$V(b) = \sigma^2 (X^T X)^{-1} = \begin{bmatrix} \frac{\sigma^2}{n} + \frac{\bar{X}^2 \sigma^2}{\sum (X - \bar{X})^2} & \frac{-\bar{X} \sigma^2}{\sum (X - \bar{X})^2} \\ \frac{-\bar{X} \sigma^2}{\sum (X - \bar{X})^2} & \frac{\sigma^2}{\sum (X - \bar{X})^2} \end{bmatrix}$$

## Section 1: Inference about $\beta_1$

1. This inference assumes a normal error regression model.
2. For a 1 unit change in the predictor, there will be a  $\beta_1$  change in mean response.

### Sampling Distribution of $b_1$

The random variable  $b_1$  is a normally distributed random variable with mean and variance given by

$$\begin{aligned} E(b_1) &= \beta_1 & b_1 &\sim \text{Normal}(\beta_1, V(\beta_1)) \\ V(b_1) &= \frac{\sigma^2}{\sum(X_i - \bar{X})^2} & \sigma^2 &= V(\epsilon) = V(Y | X) \\ &\approx \frac{s^2}{\sum(X_i - \bar{X})^2} = \frac{MSE}{\sum(X_i - \bar{X})^2}. \end{aligned}$$

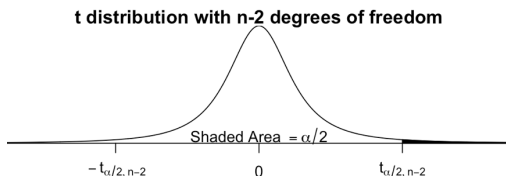
### Sampling Distribution of $t = \frac{b_1 - \beta_1}{s_{b_1}}$

The statistic  $t = \frac{b_1 - \beta_1}{s_{b_1}}$  has a  $t$  distribution with  $n - 2$  degrees of freedom where  $s_{b_1}$  is the estimated standard error of  $b_1$ .

### 100(1 - $\alpha$ )% Confidence Interval for $\beta_1$

Given a random sample of size  $n$  from a population, the 100(1 -  $\alpha$ )% confidence interval for  $\beta_1$  is given by

$$b_1 - t_{\alpha/2, n-2} s_{b_1} < \beta_1 < b_1 + t_{\alpha/2, n-2} s_{b_1}.$$



### Testing for $\beta_1$

#### Hypotheses:

$$H_0: \beta_1 = 0$$

$$H_1: \beta_1 \neq 0$$

#### Test Statistic:

$$t = \frac{b_1}{s_{b_1}}$$

#### Level $\alpha$ Rejection Rule:

Reject  $H_0$  if

- a.  $t < -t_{\alpha/2, n-2}$  or  $t > t_{\alpha/2, n-2}$
- b. p-value  $\leq \alpha$ 
  - p-value =  $2 \times \text{pt}(|t|, \text{df} = n-2, \text{lower.tail} = \text{F})$

**Example:**

The director of admissions at a college wants to describe the GPA of a freshmen at the end of their freshmen year based upon their ACT score. They will fit a simple linear model<sup>8</sup>.(Kutner)

**#### A portion of the data set**

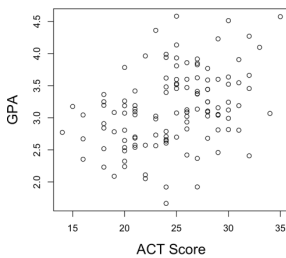
```
head(SLRSet1, n = 2)
      GPA ACT
1 2.539076 21
2 2.772057 14
```

**#### Sample Size**

```
n <- nrow(SLRSet1)
n
[1] 120
```

**#### Graph**

```
plot(GPA ~ ACT, data = SLRSet1, xlab = "ACT Score", ylab = "GPA", cex.lab = 1.5)
```

**#### Fitting Linear Model**

```
lm.fit <- lm(GPA ~ ACT, data = SLRSet1)
```

**#### Summarized Output of Fitted Model**

```
summary(lm.fit)
```

Call:

```
lm(formula = GPA ~ ACT, data = SLRSet1)
```

Residuals:

```
      Min       1Q   Median       3Q      Max
-1.44000 -0.37148 -0.04281  0.36769  1.42492
```

Coefficients:

```
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  1.89783     0.28280   6.711 7.11e-10 ***
ACT           0.05034     0.01126   4.472 1.80e-05 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Residual standard error: 0.5492 on 118 degrees of freedom

Multiple R-squared: 0.1449, Adjusted R-squared: 0.1377

F-statistic: 20 on 1 and 118 DF, p-value: 1.796e-05

**#### Confidence Interval**

```
confint(lm.fit, parm = 2, level = 0.99)
      0.5 %      99.5 %
ACT 0.02086496 0.07980892
```

**#### Hand Calculations**

```
cv <- qt(0.995, df = n - 2, lower.tail = TRUE)
b1 <- coefficients(lm.fit)[2]
b1
      ACT
0.05033694
sdres <- sd(lm.fit$residuals) * sqrt(((n - 2) + 1)/(n - 2))
sdres
[1] 0.5491597
ssx <- var(SLRSet1$ACT) * ((n - 2) + 1)
se.b1 <- sdres/sqrt(ssx)
b1 + c(-cv, cv) * se.b1
[1] 0.02086496 0.07980892
```

<sup>8</sup> Without checking, it is assumed that a normal error regression model applies.

## Section 2: Inference about $\beta_0$

1. This inference assumes a normal error regression model.
2. The mean response when the predictor is equal to zero.
3. Important when the predictors are near, or include, zero.

### Sampling Distribution of $b_0$

The random variable  $b_0$  is a normally distributed random variable with mean and variance given by

$$E(b_0) = \beta_0$$

$$b_0 \sim \text{Normal}(\beta_0, V(\beta_0))$$

$$V(b_0) = \sigma^2 \left[ \frac{1}{n} + \frac{\bar{X}^2}{\sum (X_i - \bar{X})^2} \right]$$

$$\sigma^2 = V(\epsilon) = V(Y | X)$$

$$\approx s^2 \left[ \frac{1}{n} + \frac{\bar{X}^2}{\sum (X_i - \bar{X})^2} \right] = \text{MSE} \left[ \frac{1}{n} + \frac{\bar{X}^2}{\sum (X_i - \bar{X})^2} \right].$$

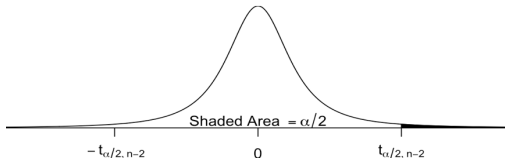
### Sampling Distribution of $t = \frac{b_0 - \beta_0}{s_{b_0}}$

The statistic  $t = \frac{b_0 - \beta_0}{s_{b_0}}$  has a  $t$  distribution with  $n - 2$  degrees of freedom where  $s_{b_0}$  is the estimated standard error of  $b_0$ .

### $100(1 - \alpha)\%$ Confidence Interval for $\beta_0$

Given a random sample of size  $n$  from a population, the  $100(1 - \alpha)\%$  confidence interval for  $\beta_0$  is given by

$$b_0 - t_{\alpha/2, n-2} s_{b_0} < \beta_0 < b_0 + t_{\alpha/2, n-2} s_{b_0}.$$



### Testing for $\beta_0$

#### Hypotheses:

$$H_0: \beta_0 = 0$$

$$H_1: \beta_0 \neq 0$$

#### Test Statistic:

$$t = \frac{b_0}{s_{b_0}}$$

#### Level $\alpha$ Rejection Rule:

Reject  $H_0$  if

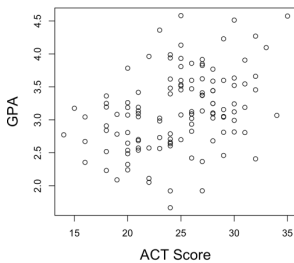
- a.  $t < -t_{\alpha/2, n-2}$  or  $t > t_{\alpha/2, n-2}$
- b.  $p\text{-value} \leq \alpha$   
 –  $p\text{-value} = 2 \times \text{pt}(|t|, \text{df} = n-2, \text{lower.tail} = \text{F})$

**Example:**

The director of admissions at a college wants to describe the GPA of a freshmen at the end of their freshmen year based upon their ACT score. They will fit a simple linear model<sup>9</sup>.(Kutner)

**#### Graph**

```
plot(GPA ~ ACT, data = SLRSet1, xlab = "ACT Score", ylab = "GPA", cex.lab = 1.5)
```

**#### Fitting Linear Model**

```
lm.fit <- lm(GPA ~ ACT, data = SLRSet1)
```

**#### Summarized Output of Fitted Model**

```
summary.fit <- summary(lm.fit)
summary.fit
```

Call:

```
lm(formula = GPA ~ ACT, data = SLRSet1)
```

Residuals:

	Min	1Q	Median	3Q	Max
Residuals	-1.44000	-0.37148	-0.04281	0.36769	1.42492

Coefficients:

	Estimate	Std. Error	t value	Pr(> t )
(Intercept)	1.89783	0.28280	6.711	7.11e-10 ***
ACT	0.05034	0.01126	4.472	1.80e-05 ***

Signif. codes: 0 '\*\*\*' 0.001 '\*\*' 0.01 '\*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.5492 on 118 degrees of freedom

Multiple R-squared: 0.1449, Adjusted R-squared: 0.1377

F-statistic: 20 on 1 and 118 DF, p-value: 1.796e-05

```
names(summary.fit)
```

[1] "call"	"terms"	"residuals"	"coefficients"
[5] "aliased"	"sigma"	"df"	"r.squared"
[9] "adj.r.squared"	"fstatistic"	"cov.unscaled"	

**#### Confidence Interval**

```
confint(lm.fit, parm = 1, level = 0.9)
      5 %      95 %
(Intercept) 1.428977 2.366683
```

**#### Hand Calculations**

```
n <- nrow(SLRSet1)
dof <- n - 2
alpha <- 0.1
cv <- qt(alpha/2, df = dof, lower.tail = FALSE)
b0 <- coefficients(summary.fit)[1]
b0
[1] 1.89783
sdres <- summary.fit$sigma
sdres
[1] 0.5491597
Xs <- 1/n + (mean(SLRSet1$ACT)^2)/(var(SLRSet1$ACT) * (n - 1))
se.b0 <- sdres * sqrt(Xs)
b0 + c(-cv, cv) * se.b0
[1] 1.428977 2.366683
```

<sup>9</sup> Without checking, it is assumed that a normal error regression model applies.

### Section 3: Interval Estimation of $E[Y_h]$

#### Assumptions:

1. This inference assumes a normal error regression model.
2. Let  $X_i, i = 1, 2, \dots, n$  be the observed values of the predictor variable.
3. Let  $X_h, h = 1, 2, \dots, H$  be values for the predictor variable where one wants to estimate the mean response  $E(Y | X_h)$ .

#### Definition:

The point estimate of mean response at  $X_h$ ,  $E[Y_h | X_h] = \beta_0 + \beta_1 X_h$ , is  $\hat{Y}_h = b_0 + b_1 X_h$ .

#### Sampling Distribution of $\hat{Y}_h$

The random variable  $\hat{Y}_h$  is a normally distributed random variable with mean and variance given by

$$\begin{aligned} E[\hat{Y}_h | X_h] &= E[Y_h] & \hat{Y}_h &\sim \text{Normal}(E[\hat{Y}_h | X_h], V[\hat{Y}_h | X_h]) \\ V[\hat{Y}_h | X_h] &= \sigma^2 \left[ \frac{1}{n} + \frac{(X_h - \bar{X})^2}{\sum (X_i - \bar{X})^2} \right] & \sigma^2 &= V(\epsilon) = V(Y | X) \\ &\approx s^2 \left[ \frac{1}{n} + \frac{(X_h - \bar{X})^2}{\sum (X_i - \bar{X})^2} \right] = MSE \left[ \frac{1}{n} + \frac{(X_h - \bar{X})^2}{\sum (X_i - \bar{X})^2} \right]. \end{aligned}$$

#### Controlling Size of Variance:

1. For any  $n$ ,  $V[\hat{Y}_h | X_h] \geq \sigma^2 \left[ \frac{(X_h - \bar{X})^2}{\sum (X_i - \bar{X})^2} \right]$ .
2. If  $X_h = \bar{X}$ ,  $V[\hat{Y}_h | X_h = \bar{X}] = \frac{\sigma^2}{n}$ .
3. The size of  $V[\hat{Y}_h | X_h]$  depends on values that can be selected:
  - Select  $X_h$  near  $\bar{X}$
  - Select  $X_i$  so that  $\sum (X_i - \bar{X})^2$  is large.

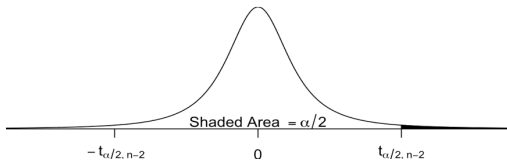
#### Sampling Distribution of $t$

The statistic  $t = \frac{\hat{Y}_h - E[Y_h]}{s_{\hat{Y}_h}}$  has a  $t$  distribution with  $n - 2$  degrees of freedom where  $s_{\hat{Y}_h}$  is the estimated standard error of  $s_{\hat{Y}_h}$ .

#### 100(1 - $\alpha$ )% Confidence Interval for $E[Y_h | X_h]$

Given a random sample of size  $n$  from a population, the 100(1 -  $\alpha$ )% confidence interval for  $E[Y_h | X_h]$  is given by

$$\hat{Y}_h - t_{\alpha/2, n-2} s_{\hat{Y}_h} < E[Y_h | X_h] < \hat{Y}_h + t_{\alpha/2, n-2} s_{\hat{Y}_h}.$$





## Section 4: Prediction from a New Observation

If a new observation is to be collected, predict the individual response.

### Assumptions:

1. This inference assumes a normal error regression model.
2. Let  $X_i, i = 1, 2, \dots, n$  be the observed values of the predictor variable.
3. Let  $X_h, h = 1, 2, \dots, H$  be values for the predictor variable where one wants to predict the response  $Y_{h(new)}$  if additional observations were to be taken.

### Definition:

If an additional observation is taken at  $X_h$ , then predicted response,  $Y_{h(new)} = \beta_0 + \beta_1 X_h + \epsilon_h$ , is  $Y_{h(new)_h} = b_0 + b_1 X_h$ .

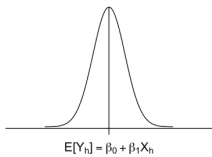
- $Y_{h(new)}$  is not a parameter
- $Y_{h(new)}$  is random variable.

### Sampling Distribution of $\frac{Y_h - \hat{Y}_h}{s_{pred}}$

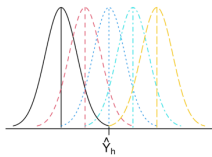
The random variable  $\frac{Y_{h(new)} - \hat{Y}_h}{s_{pred}}$  has a  $t$  distribution with  $n - 2$  degrees of freedom.

$$V(pred) = \sigma^2 + V(\hat{Y}_h)$$

Known Parameters:  $\beta_0, \beta_1$  and  $\sigma^2$



Unknown Parameters:  $\beta_0, \beta_1$



### 100(1 - $\alpha$ )% Prediction Interval for $Y_{h(new)}$

Given a sample of size  $n$  from a population that satisfies the normal error regression model, a 100(1 -  $\alpha$ )% prediction interval for  $Y_h$  is given by

$$\hat{Y}_h - t_{\alpha/2, n-2} s_{pred} < Y_{h(new)} < \hat{Y}_h + t_{\alpha/2, n-2} s_{pred}.$$

## Section 5: Example

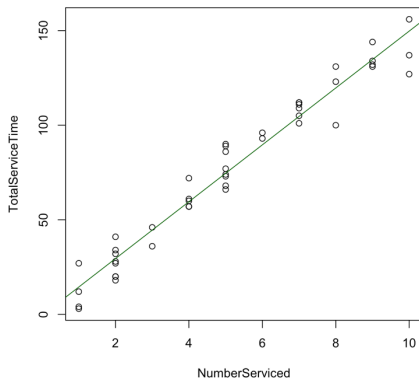
CopyCo rents office copiers. As part of a copier rental, CopyCo provides preventative maintenance and repair services. The collected data is for forty-five recent preventative maintenance visits. For each visit, the number of copiers serviced was recorded, as well as the total service time per visit<sup>10</sup>. (Kutner)

1. Does there appear to be a linear relationship between the number of copiers serviced and the total service time per visit?

```
#### Partial Data Frame
head(CopyCo)
  TotalServiceTime NumberServiced
1             20             2
2             60             4
3             46             3
4             41             2
5             12             1
6            137            10
n <- nrow(CopyCo)

#### Fitting Linear Model
lm.fit <- lm(TotalServiceTime ~ NumberServiced, data = CopyCo)

#### Graph
plot(CopyCo[2:1])
abline(coefficients(lm.fit), col = "darkgreen")
```



2. Estimate the change in the average service time when the number copiers being serviced increases by 1.

```
#### Summarized Output of Fitted Model
summary.fit <- summary(lm.fit)
summary.fit

Call:
lm(formula = TotalServiceTime ~ NumberServiced, data = CopyCo)

Residuals:
    Min       1Q   Median       3Q      Max
-22.7723  -3.7371   0.3334   6.3334  15.4039

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  -0.5802     2.8039  -0.207   0.837
NumberServiced 15.0352     0.4831  31.123 <2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 8.914 on 43 degrees of freedom
Multiple R-squared:  0.9575,    Adjusted R-squared:  0.9565
F-statistic: 968.7 on 1 and 43 DF,  p-value: < 2.2e-16

#### Confidence Interval
confint(lm.fit, parm = 2, level = 0.9)
              5 %      95 %
NumberServiced 14.22314 15.84735
```

<sup>10</sup> Without checking, it is assumed that a normal error regression model applies.

3. The manufacturer of the copy machines rented by CopyCo advertises that the average total service time should not increase by more than 14 minutes for each additional copier serviced during a service visit.

#### #### Summarized Output of Fitted Model

```
names(summary.fit)
[1] "call"          "terms"          "residuals"      "coefficients"
[5] "aliased"        "sigma"          "df"             "r.squared"
[9] "adj.r.squared" "fstatistic"     "cov.unscaled"
```

```
summary.fit$coefficients
              Estimate Std. Error    t value    Pr(>|t|)
(Intercept)  -0.5801567  2.8039411  -0.2069076  8.370587e-01
NumberServiced 15.0352480  0.4830872  31.1232581  4.009032e-31
```

#### #### Test Statistic

```
b1 <- summary.fit$coefficients[2, 1]
b1
[1] 15.03525
se.b1 <- summary.fit$coefficients[2, 2]
se.b1
[1] 0.4830872
hypothesized.value <- 14
```

```
t <- (b1 - hypothesized.value)/se.b1
t
[1] 2.142984
```

#### #### Critical Values

```
dof <- n - 2
qt(0.05, df = dof, lower.tail = FALSE)
[1] 1.681071
```

#### #### Test Statistic

```
pt(t, df = dof, lower.tail = FALSE)
[1] 0.01890766
```

4. Confidence and Prediction Intervals when  $X_h = 5, 6$

#### #### Predictor Values

```
X_h <- data.frame(NumberServiced = c(5, 6))
```

#### #### Confidence Intervals

```
predict(lm.fit, newdata = X_h, interval = "confidence", level = 0.9)
      fit      lwr      upr
1 74.59608 72.36054 76.83162
2 89.63133 87.28387 91.97880
```

#### #### Prediction Intervals

```
predict(lm.fit, newdata = X_h, interval = "prediction", se.fit = TRUE)
$fit
      fit      lwr      upr
1 74.59608 56.42133 92.77084
2 89.63133 71.43628 107.82639
```

```
$se.fit
      1      2
1.329831 1.396411
```

```
$df
[1] 43
```

```
$residual.scale
[1] 8.913508
```

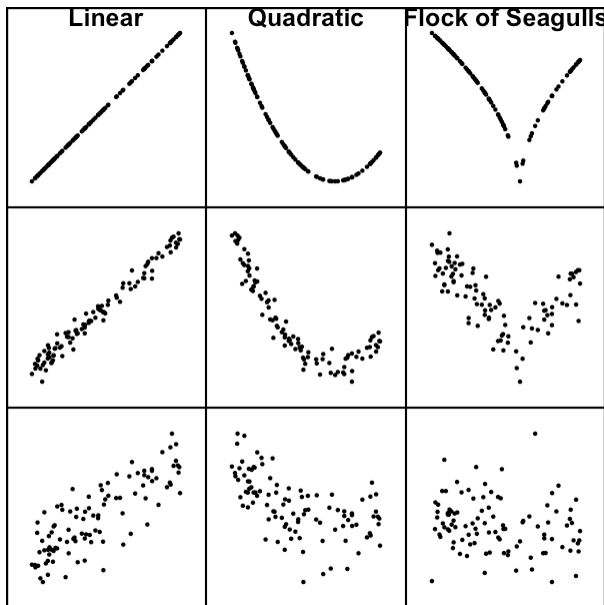
#### #### Variance/Covariance Matrix

```
var(CopyCo)
              TotalServiceTime NumberServiced
TotalServiceTime      1826.7455      116.333333
NumberServiced        116.3333       7.737374
mean(CopyCo$NumberServiced)
[1] 5.111111
```

## Section 6: Covariance & Pearson Correlation Coefficient

### Definition:

Two numerical variables  $X$  and  $Y$  are called **correlated** if they are associated.



### Definition:

The **covariance** of random variables  $X$  and  $Y$  is  $Cov(X, Y) = E[(X - \mu_X)(Y - \mu_Y)]$ . Covariance measures the tendency of two random variables to change together along a straight line.

### Definition:

The **linear correlation coefficient** of random variables  $X$  and  $Y$  is  $\rho_{X,Y} = \frac{Cov(X,Y)}{\sigma_X \sigma_Y}$ . Correlation measures the strength and direction of the linear association between two variables.

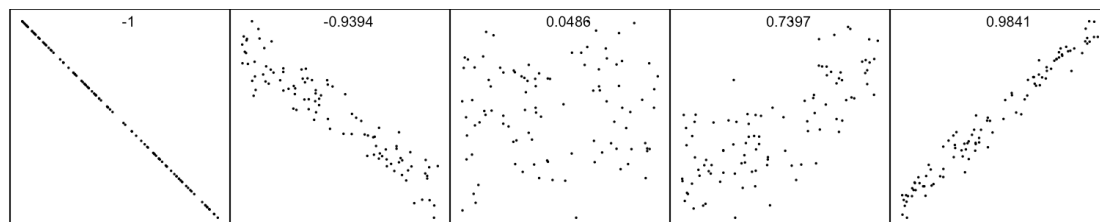
### Point Estimates

Given a random sample  $(x_i, y_i)$  of size  $n$ , the estimates are as follows:

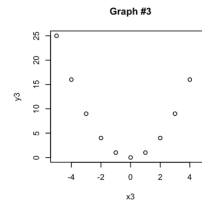
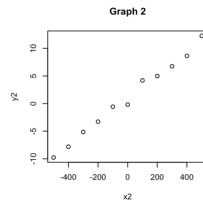
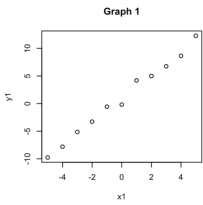
$$cov(x, y) = \frac{\sum (x - \bar{x})(y - \bar{y})}{n - 1} \qquad r = \frac{cov(x, y)}{s_x s_y}$$

### Facts about Covariance and Correlation

1. Linear correlation coefficient is bounded above by 1 and below by -1.



## 2. The scale of observations affects size of covariance, but it does not affect the size of correlation



### #### Graph 1 Data

```
x1 <- -5:5
ln <- length(x1)
error <- rnorm(ln)
y1 <- 2 * x1 + 1 + error
cov(x1, y1)
[1] 22.49821
cor(x1, y1)
[1] 0.9836314
```

### #### Graph #2 Data

```
x2 <- x1 * 100
y2 <- 100 * y1
cov(x2, y2)
[1] 224982.1
cor(x2, y2)
[1] 0.9836314
```

## 3. Linear correlation and covariance only measure straight line relationships.

### #### Graph #3 Data

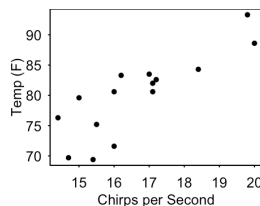
```
x3 <- -5:5
y3 <- x3^2

cor(x3, y3)
[1] 0
```

## 4. If two random variables $X$ and $Y$ are independent, then $\text{Cov}(X,Y)$ and $\rho_{X,Y}$ equal zero. (But not necessarily the other way around.)

### Example:

The temperature and the number of times a cricket chirped per second from “The Song of Insects” by Dr.G.W. Pierce.



### #### Partial Dataframe

```
head(chirps, n = 2)
  Chirps Temp
1     20 88.6
2     16 71.6
```

### #### Variance/Covariance Matrix

```
cov(chirps)
      Chirps      Temp
Chirps 2.896952  9.534143
Temp   9.534143 44.988286
```

### #### Correlation Matrix

```
cor(chirps)
      Chirps      Temp
Chirps 1.0000000 0.8351438
Temp   0.8351438 1.0000000
```



## Chapter 4: Multiple Linear Regression

### Section 1: General Linear Model with normal error

**Definition:**

A **general linear regression model with normal error** relates the response variable  $Y_i$  and  $p - 1$  predictor variables  $X_1, X_2, \dots, X_{p-1}$  as follows:

$$\begin{aligned} Y_i &= \beta_0 + \beta_1 X_{i,1} + \beta_2 X_{i,2} + \dots + \beta_{p-1} X_{i,p-1} + \epsilon_i \\ &= \beta_0 + \sum_{j=1}^{p-1} \beta_j X_{i,j} + \epsilon_i \end{aligned}$$

where

1.  $Y_i$  is the value of the response in the  $i^{th}$  trial
2.  $\beta_0, \beta_1, \dots, \beta_{p-1}$  are parameters
3.  $X_{i,j}$  is the value of the  $j^{th}$  predictor in the  $i^{th}$  trial, and is a known constant.
4.  $\epsilon_i$  are independent Normally distributed random variables with mean 0 and variance  $\sigma^2$ .

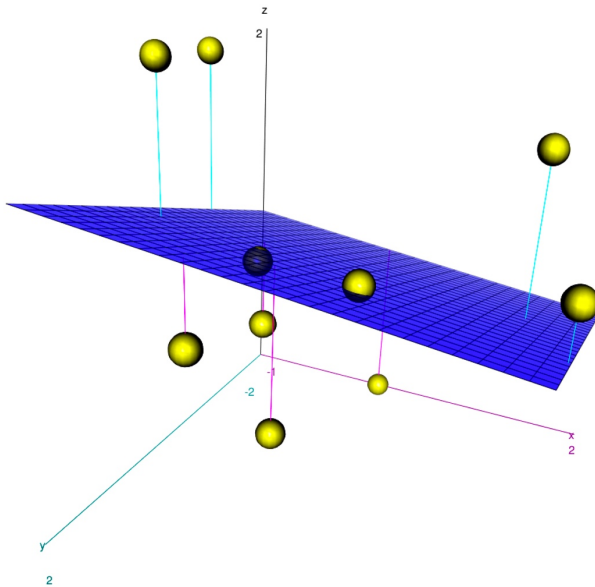
$$Y = \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{bmatrix} \quad X = \begin{bmatrix} 1 & X_{1,1} & X_{1,2} & \dots & X_{1,p-1} \\ 1 & X_{2,1} & X_{2,2} & \dots & X_{2,p-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & X_{n,1} & X_{n,2} & \dots & X_{n,p-1} \end{bmatrix} \quad \beta = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_{p-1} \end{bmatrix} \quad \epsilon = \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{bmatrix}$$

**Definition:**

A **case** is a collection of values for the predictor variables and possibly the response variable.<sup>11</sup>

- a. Predictors only:  $(X_1, X_2, \dots, X_{p-1})$ .
  - The vector  $X_i = [X_{i,1}, X_{i,2}, \dots, X_{i,j}, \dots, X_{i,p-1}]^T$  may be referred to as the  $i^{th}$  case or  $i^{th}$  observation on the predictors.
- b. Predictors and Response:  $(X_1, X_2, \dots, X_{p-1}, Y)$

Data: (1,0,2.5,-11.7) (3,5,6.4,-21) (4,2.4,9.6,-51.3) (7,1.7,5.5,-19) (1.5,10,9.8,-33.4) (6.2,9,5.1,4.1)



<sup>11</sup> Context should make the difference clear.

### Regression Coefficients

$\beta_j$  represents the change in  $E(Y)$  with a one unit change in  $X_j$  when all other variables are held constant.<sup>12</sup>

$$\begin{aligned} E[Y | X_j + 1] &= \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_j (X_j + 1) + \cdots + \beta_{p-1} X_{p-1} \\ E[Y | X_j] &= \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_j X_j + \cdots + \beta_{p-1} X_{p-1} \\ E[Y | X_j + 1] - E[Y | X_j] &= \beta_j \end{aligned}$$

### $p - 1$ predictors

$$Y_i = \beta_0 + \beta_1 X_{i,1} + \beta_2 X_{i,2} + \cdots + \beta_{p-1} X_{i,p-1} + \epsilon_i$$

There are  $p$  parameters:  $\beta_0, \beta_1, \beta_2, \dots, \beta_j, \dots, \beta_{p-1}$ . Since  $\beta_0$  is the intercept, so it doesn't get a predictor. Thus, there are  $p - 1$  predictors in this standard model.

### Qualitative Predictors

#### **Definition:**

A **qualitative predictor** is a predictor variable that represents categories and not numerical values.

#### **Definition:**

An **indicator variable** is a variable that indicates that an outcome  $A$  has occurred, or not occurred, by taking a value of one, or zero, respectively.

$$X_A = \begin{cases} 1 & \text{if } A \text{ occurred} \\ 0 & \text{otherwise} \end{cases}$$

A qualitative predictor variable with  $c$  categories is represented by  $c - 1$  indicator variables.

#### **Example:**

A qualitative predictor measures satisfaction. Its possible categories: Low, Medium, High.

$$X_{Medium} = \begin{cases} 1 & \text{Medium} \\ 0 & \text{Otherwise} \end{cases} \quad X_{High} = \begin{cases} 1 & \text{High} \\ 0 & \text{Otherwise} \end{cases}$$

#### **Definition:**

The **reference** is the category that all others are generally compared to. It will be the category that is not represented by any indicator.

<sup>12</sup> Situations arise where this interpretation does not hold. This occurs when predictors are related in some way. In that case, a change in one predictor can't be made without another predictor also changing.



Multiple Linear Regression Techniques can be applied to many situations. Usually, this is done with a suitable substitution of variables.

### Polynomial Regression

Suppose the relationship between the response and a single predictor looks to follow a polynomial with degree  $k > 1$ .

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_1^2 + \cdots + \beta_j X_1^j + \cdots + \beta_k X_1^k + \epsilon$$

A substitution of variables turns this into a multiple linear regression problem.

Substituting  $Z_1 = X_1, Z_2 = X_1^2, \dots, Z_j = X_1^j, \dots, Z_k = X_1^k$  will result in a relationship<sup>13</sup> such as

$$Y = \beta_0 + \beta_1 Z_1 + \beta_2 Z_2 + \beta_3 Z_3 + \beta_4 Z_4 + \epsilon.$$

### Transformed Variables

$$\text{A: } \log(Y_i) = \beta_0 + \sum_{j=1}^{p-1} \beta_j X_{ij} + \epsilon_i \quad \text{B: } Y_i = \frac{1}{\beta_0 + \beta_1 X_{i,1} + \beta_2 X_{i,2} + \cdots + \beta_{p-1} X_{i,p-1} + \epsilon_i}$$

A: Substituting  $Y^* = \log(Y_i)$  yields  $Y^* = \beta_0 + \sum_{j=1}^{p-1} \beta_j X_{ij} + \epsilon_i$

B: Substituting  $Y^* = \frac{1}{Y_i}$  yields  $Y^* = \beta_0 + \beta_1 X_{i,1} + \beta_2 X_{i,2} + \cdots + \beta_{p-1} X_{i,p-1} + \epsilon_i$

### Interactions Effects

#### **Definition:**

An **interaction** between predictor is present when the change in the response based on a change in one predictor is dependent on the value of another predictor.

$$\begin{aligned} Y &= \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_1 X_2 + \epsilon_i \\ &= \beta_0 + \beta_1 Z_1 + \beta_2 Z_2 + \beta_3 Z_3 + \epsilon_i \end{aligned}$$

$$\begin{aligned} Z_1 &= X_1 \\ Z_2 &= X_2 \\ Z_3 &= X_1 X_2 \end{aligned}$$

#### **Example:**

Suppose  $E[Y | X_1, X_2] = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_1 X_2$  where  $X_1, X_2$  are two indicator variables and  $\beta_1, \beta_2$  and  $\beta_3$  are all nonzero.

$$X_1 = \begin{cases} 1 & \text{Success Type 1} \\ 0 & \text{Otherwise} \end{cases} \quad X_2 = \begin{cases} 1 & \text{Success Type 2} \\ 0 & \text{Otherwise} \end{cases}$$

$$E[Y | X_1, X_2] = \begin{cases} \beta_0 & X_1 = 0, X_2 = 0 \\ \beta_0 + \beta_1 & X_1 = 1, X_2 = 0 \\ \beta_0 + \beta_2 & X_1 = 0, X_2 = 1 \\ \beta_0 + \beta_1 + \beta_2 + \beta_3 & X_1 = 1, X_2 = 1 \end{cases}$$

<sup>13</sup> The drawback here is that the interpretation of a  $\beta_j$  will not be the same. It is not possible to hold all except one  $Z_j$  variable constant. They all change together.

## Section 2: Estimation of Parameters

### Definition:

Given a data set  $(X_{1,1}, X_{2,1}, \dots, X_{p-1,1}, Y_1), (X_{1,2}, X_{2,2}, \dots, X_{p-1,2}, Y_2), \dots, (X_{1,n}, X_{2,n}, \dots, X_{p-1,n}, Y_n)$ , the **method of least squares** estimates the intercept  $\beta_0$  and slope  $\beta_i, i = 1, 2, \dots, p - 1$  parameters. It works by minimizing the function

$$\begin{aligned} SS(b_0^*, b_1^*, \dots, b_{p-1}^*) &= \sum_{i=1}^n [Y_i - (b_0^* + b_1^* X_{i,1} + b_2^* X_{i,2} + \dots + b_{p-1}^* X_{i,p-1})]^2 \\ &= (Y - Xb^*)^T (Y - Xb^*) \end{aligned}$$

The values of  $b_0^*, b_1^*, \dots, b_{p-1}^*$  that minimize  $SS(b_0^*, b_1^*, \dots, b_{p-1}^*)$  will be denoted by  $b_0, b_1, \dots, b_{p-1}$ .

- $b_0$  will be called the **least squares estimate** of the intercept  $\beta_0$ .
- $b_i, i = 1, 2, \dots, p - 1$  will be called the **least squares estimate** of the slope  $\beta_i$ .

$$SS(b_0, b_1, \dots, b_{p-1}) \leq \min_{\substack{\text{all intercepts } b_0^* \\ \text{all slopes } b_1^*, \dots, b_{p-1}^*}} SS(b_0^*, b_1^*, \dots, b_{p-1}^*)$$

$$X = \begin{bmatrix} 1 & X_{1,1} & X_{1,2} & \dots & X_{1,p-1} \\ 1 & X_{2,1} & X_{2,2} & \dots & X_{2,p-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & X_{n,1} & X_{n,2} & \dots & X_{n,p-1} \end{bmatrix} \quad X^T X b = X^T Y \quad b = (X^T X)^{-1} X^T Y = \begin{bmatrix} b_0 \\ b_1 \\ \vdots \\ b_{p-1} \end{bmatrix} \quad E(b) = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_{p-1} \end{bmatrix}$$

### Point Estimate of the Mean Response

#### Definition:

The **mean response function** at  $X_1, X_2, \dots, X_{p-1}$  is given by  $E[Y | X_1, X_2, \dots, X_{p-1}] = \beta_0 + \beta_1 X_1 + \dots + \beta_{p-1} X_{p-1}$ .

The **equation of the least squares regression function** is given by  $\hat{Y} = b_0 + b_1 X_1 + b_2 X_2 + \dots + b_{p-1} X_{p-1}$ , where  $b_0, b_1, \dots, b_{p-1}$  are unbiased estimates of  $\beta_0, \beta_1, \dots, \beta_{p-1}$ .

The estimates of the mean response at the observed cases of  $(X_{i,1}, X_{i,2}, \dots, X_{i,p-1})$  is given by evaluating the equation of the least squares regression function at  $(X_{i,1}, X_{i,2}, \dots, X_{i,p-1})$ .

$$\begin{aligned} \hat{Y} &= \begin{bmatrix} \hat{Y}_1 \\ \hat{Y}_2 \\ \vdots \\ \hat{Y}_n \end{bmatrix} = \begin{bmatrix} 1 & X_{1,1} & X_{1,2} & \dots & X_{1,p-1} \\ 1 & X_{2,1} & X_{2,2} & \dots & X_{2,p-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & X_{n,1} & X_{n,2} & \dots & X_{n,p-1} \end{bmatrix} \begin{bmatrix} b_0 \\ b_1 \\ \vdots \\ b_{p-1} \end{bmatrix} \\ &= Xb \\ &= X(X^T X)^{-1} X^T Y = HY \end{aligned}$$

$$H = X(X^T X)^{-1} X^T \quad (\text{hat matrix})$$

When  $(X_{i,1}, X_{i,2}, \dots, X_{i,p-1})$  is one of the observed cases of predictors, the **mean response** at this case is also called a **fitted value**.

## Residuals

### **Definition:**

The  $i^{th}$  **residual**  $e_i$  is the difference between the  $i^{th}$  observed value and the  $i^{th}$  fitted value. That is,  $e_i = Y_i - \hat{Y}_i$ .

$$e = \begin{bmatrix} e_1 \\ e_2 \\ \vdots \\ e_n \end{bmatrix} = \begin{bmatrix} Y_1 - \hat{Y}_1 \\ Y_2 - \hat{Y}_2 \\ \vdots \\ Y_n - \hat{Y}_n \end{bmatrix} = \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{bmatrix} - \begin{bmatrix} \hat{Y}_1 \\ \hat{Y}_2 \\ \vdots \\ \hat{Y}_n \end{bmatrix} = Y - \hat{Y}$$

### **Notes about residuals:**

1.  $e$  is a random vector
2.  $e_i$  estimate  $\epsilon_i$
3.  $e_i$  are dependent.
4.  $e = (I - H)Y$

$$V(e) = \sigma^2(I - H)$$

5.  $V(e)$  is a variance/covariance matrix.
  - a.  $V(e)_{i,j} = V(e_i)$  for  $i = j$
  - b.  $V(e)_{i,j} = Cov(e_i, e_j)$  for  $i \neq j$

## Estimating the Variance of the Error

$$SSE = \sum (Y_i - \hat{Y}_i)^2$$

$$DFE = n - p$$

$$s^2 = \frac{SSE}{DFE}$$

## Properties of the Fitted Regression

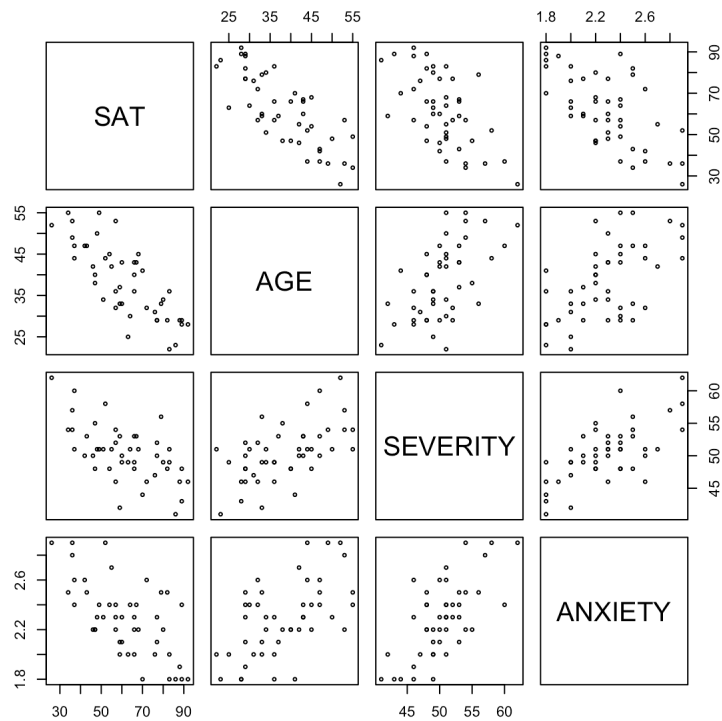
1. The sum of the residuals is zero.
2. The sum of the squared residuals is a minimum.
3. The sum of the observed values is equal to the sum of the fitted values.
4. The sum of the weighted residuals is zero, when the weight on the  $i^{th}$  residual is  $X_i$ .
5. The sum of the weighted residuals is zero, when the weight on the  $i^{th}$  residual is  $\hat{Y}_i$ .

Example

A hospital administrator wished to study the relationship between patient satisfaction  $Y$  and patient's age  $X_1$ , severity of illness  $X_2$ , and anxiety level  $X_3$ . The administrator randomly selected 46 patients. The data is held in the PatSat dataset. Larger values for  $Y, X_2$  and  $X_3$  indicate higher satisfaction, severity and anxiety. (Kutner)

```
#### Partial Dataframe
head(PatSat)
  SAT AGE SEVERITY ANXIETY
1  48  50      51    2.3
2  57  36      46    2.3
3  66  40      48    2.2
4  70  41      44    1.8
5  89  28      43    1.8
6  36  49      54    2.9

#### Scatterplot Matrix
pairs(PatSat, cex = 0.5)
```



```
#### Variance/Covariance Matrix
var(PatSat)
      SAT      AGE  SEVERITY  ANXIETY
SAT    297.095652 -120.937198 -44.8289855 -3.32579710
AGE   -120.937198  79.532367  21.8483092  1.52077295
SEVERITY -44.828986  21.848309  18.6067633  0.86579710
ANXIETY  -3.325797  1.520773  0.8657971  0.08960386

#### Correlation Matrix
cor(PatSat)
      SAT      AGE  SEVERITY  ANXIETY
SAT    1.0000000 -0.7867555 -0.6029417 -0.6445910
AGE   -0.7867555  1.0000000  0.5679505  0.5696775
SEVERITY -0.6029417  0.5679505  1.0000000  0.6705287
ANXIETY  -0.6445910  0.5696775  0.6705287  1.0000000
```

#### #### Fitting Linear Model

```
satisfaction.fit <- lm(SAT ~ AGE + SEVERITY + ANXIETY, data = PatSat)
```

#### #### Components of Fitted Model

```
names(satisfaction.fit)
[1] "coefficients" "residuals"      "effects"        "rank"
[5] "fitted.values" "assign"          "qr"             "df.residual"
[9] "xlevels"       "call"           "terms"          "model"
```

```
satisfaction.fit$df.residual
[1] 42
```

#### #### Summarized Output of Fitted Model

```
satisfaction.summary <- summary(satisfaction.fit)
satisfaction.summary
```

Call:

```
lm(formula = SAT ~ AGE + SEVERITY + ANXIETY, data = PatSat)
```

Residuals:

	Min	1Q	Median	3Q	Max
	-18.3524	-6.4230	0.5196	8.3715	17.1601

Coefficients:

	Estimate	Std. Error	t value	Pr(> t )	
(Intercept)	158.4913	18.1259	8.744	5.26e-11	***
AGE	-1.1416	0.2148	-5.315	3.81e-06	***
SEVERITY	-0.4420	0.4920	-0.898	0.3741	
ANXIETY	-13.4702	7.0997	-1.897	0.0647	.

---

Signif. codes: 0 '\*\*\*' 0.001 '\*\*' 0.01 '\*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 10.06 on 42 degrees of freedom

Multiple R-squared: 0.6822, Adjusted R-squared: 0.6595

F-statistic: 30.05 on 3 and 42 DF, p-value: 1.542e-10

#### #### Components of Summary

```
names(satisfaction.summary)
[1] "call"          "terms"         "residuals"     "coefficients"
[5] "aliased"       "sigma"         "df"            "r.squared"
[9] "adj.r.squared" "fstatistic"    "cov.unscaled"
```

#### #### Residual Standard Error (s)

```
satisfaction.summary$sigma
[1] 10.05798
```

#### #### Fitted Values

```
satisfaction.fit$fitted.values[1:2]
      1      2
47.88707 66.07965
```

#### #### Hand Computations of Fitted Values

```
X <- as.matrix(cbind(rep(1, nrow(PatSat)), PatSat[2:4]))
```

```
b <- solve(t(X) %*% X) %*% t(X) %*% PatSat[[1]]
```

b

	[,1]
rep(1, nrow(PatSat))	158.4912517
AGE	-1.1416118
SEVERITY	-0.4420043
ANXIETY	-13.4701632

```
(X %*% b)[1:2]
```

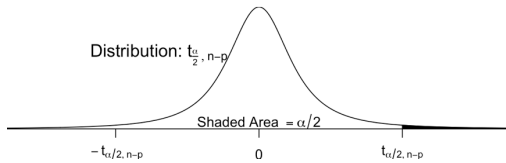
```
[1] 47.88707 66.07965
```

### Section 3: Inference with Multiple Slope Parameters

1. This inference assumes a normal error regression model.
2. Holding all other variables constant, for a 1 unit change in  $X_i$ , there will be a  $\beta_k, k > 0$  change in mean response.
3.  $V(b) = \sigma^2(X^T X)^{-1}$  is a variance/covariance matrix.
  - a.  $V(b)_{i,j} = V(b_i)$  for  $i = j$
  - b.  $V(b)_{i,j} = Cov(b_i, b_j)$  for  $i \neq j$

#### Sampling Distribution of $t = \frac{b_k - \beta_k}{s_{b_k}}$

The statistic  $t = \frac{b_k - \beta_k}{s_{b_k}}$  has a  $t$  distribution with  $n - p$  degrees of freedom where  $s_{b_k}$  is the estimated standard error of  $b_k$ .



#### Tests for $\beta_k$

If all other variables are included, is  $\beta_k = 0$  or not?

##### Hypotheses:

$$H_0: \beta_k = 0$$

$$H_1: \beta_k \neq 0$$

##### Test Statistic:

$$t = \frac{b_k}{s_{b_k}}$$

##### Level $\alpha$ Rejection Rule:

Reject  $H_0$  if

- a.  $t < -t_{\alpha/2, n-p}$  or  $t > t_{\alpha/2, n-p}$
- b.  $p\text{-value} \leq \alpha$ 
  - $p\text{-value} = 2 \times \text{pt}(|t|, \text{df} = n-p, \text{lower.tail} = F)$

#### Interval Estimation of $\beta_k$

Given a random sample of size  $n$  from a population, the  $100(1 - \alpha)\%$  confidence interval for  $\beta_k$  is given by

$$b_k - t_{\alpha/2, n-p} s_{b_k} < \beta_k < b_k + t_{\alpha/2, n-p} s_{b_k}.$$

#### Joint Inferences (Bonferroni Correction)

To estimate  $2 \leq g \leq p$  coefficients simultaneously, use  $g$  confidence intervals given by  $b_k \pm t_{\alpha/2g, n-p} s_{b_k}$ .

- To make  $P(\text{all intervals are correct}) \geq 1 - \alpha$ , each individual interval should have a confidence level of  $100 \times \left(1 - \frac{\alpha}{2g}\right)\%$ .
- To make  $P(\text{no type I errors}) \leq \alpha$ , each individual two-sided test should have a significance level of  $\frac{\alpha}{2g}$ .

##### Example:

Suppose you want to compute a confidence interval of  $\beta_0, \beta_2$  and  $\beta_6$ . Additionally, you want a **simultaneous** confidence level of 98%. What confidence level would you use for each individual confidence interval.

## Interval Estimation of $E(Y_h)$

### Assumptions:

1. This inference assumes a normal error regression model.
2. The mean response at predictor vector  $X_h$  is given by evaluating the regression equation at  $X_h$ , namely

$$E[Y_h|X_h] = \beta_0 + \beta_1 X_{h,1} + \cdots + \beta_{h,p-1} X_{h,p-1}.$$

3. The estimate of the mean response at predictor vector  $X_h$  is given by evaluating the equation of the least squares regression function at  $X_h$ , namely

$$\hat{Y}_h = b_0 + b_1 X_{h,1} + \cdots + b_{h,p-1} X_{h,p-1}.$$

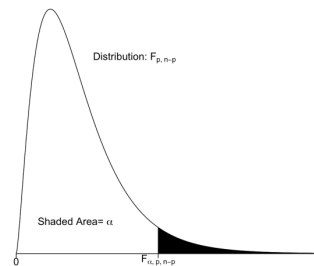
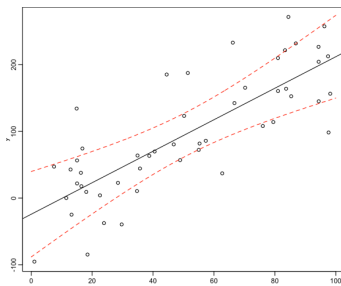
$$X_h = \begin{bmatrix} 1 \\ X_{h,1} \\ \vdots \\ X_{h,p-1} \end{bmatrix} \quad b = \begin{bmatrix} b_0 \\ b_1 \\ \vdots \\ b_{p-1} \end{bmatrix} \quad \hat{Y}_h = X_h^T b \quad \hat{Y}_h \pm t_{\alpha/2, n-p} S_{\hat{Y}_h} \quad V(\hat{Y}_h) = X_h^T V(b) X_h = \sigma^2 X_h^T (X^T X)^{-1} X_h$$

## Confidence Band/Region for Regression Function

Compute confidence intervals for **all**  $X_h$  simultaneously using

$$\hat{Y}_h \pm W S_{\hat{Y}_h}.$$

- a.  $W^2 \sim p F_{\alpha, p, n-p}$
- b.  $F_{\alpha, p, n-p}$  is a critical value take from an  $F$  distribution with degrees of freedom  $df1 = p, df2 = n - p$ .



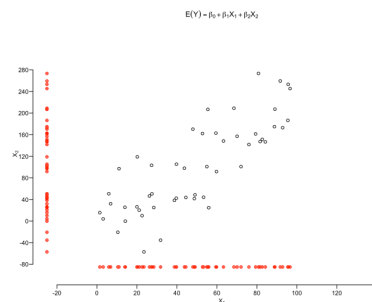
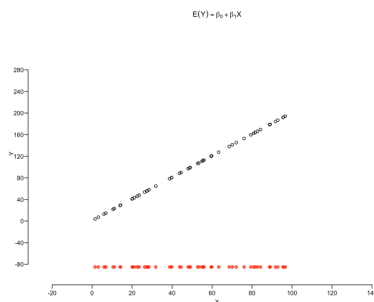
## Prediction of $Y_{h(new)}$

$$V(pred) = \sigma^2 + V(\hat{Y}_h) \quad \hat{Y}_h - t_{\alpha/2, n-p} S_{pred} < Y_{h(new)} < \hat{Y}_h + t_{\alpha/2, n-p} S_{pred}$$

## Scope & Extrapolation

### Definitions:

The **scope** of a dataset is the range of observed predictors. **Extrapolation** occurs when the the mean response is estimated/predicted outside the scope of the observed data.



## Example

A hospital administrator wished to study the relationship between patient satisfaction  $Y$  and patient's age  $X_1$ , severity of illness  $X_2$ , and anxiety level  $X_3$ . The administrator randomly selected 46 patients. The data is held in the PatSat dataset. Larger values for  $Y$ ,  $X_2$  and  $X_3$  indicate higher satisfaction, severity and anxiety. (K)

```
#### Partial Dataframe
head(PatSat, n = 3)
  SAT AGE SEVERITY ANXIETY
1  48  50      51    2.3
2  57  36      46    2.3
3  66  40      48    2.2

#### Fitting Linear Model
satisfaction.fit <- lm(SAT ~ AGE + SEVERITY + ANXIETY, data = PatSat)

#### Components of Fitted Model
names(satisfaction.fit)
[1] "coefficients" "residuals"      "effects"        "rank"
[5] "fitted.values" "assign"         "qr"             "df.residual"
[9] "xlevels"      "call"          "terms"         "model"

#### Summarized Output of Fitted Model
satisfaction.summary <- summary(satisfaction.fit)
satisfaction.summary

Call:
lm(formula = SAT ~ AGE + SEVERITY + ANXIETY, data = PatSat)

Residuals:
    Min       1Q   Median       3Q      Max
-18.3524  -6.4230   0.5196   8.3715  17.1601

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  158.4913    18.1259   8.744 5.26e-11 ***
AGE          -1.1416     0.2148  -5.315 3.81e-06 ***
SEVERITY     -0.4420     0.4920  -0.898  0.3741
ANXIETY     -13.4702     7.0997  -1.897  0.0647 .
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 10.06 on 42 degrees of freedom
Multiple R-squared:  0.6822,    Adjusted R-squared:  0.6595
F-statistic: 30.05 on 3 and 42 DF,  p-value: 1.542e-10

names(satisfaction.summary)
[1] "call"          "terms"          "residuals"      "coefficients"
[5] "aliased"       "sigma"          "df"             "r.squared"
[9] "adj.r.squared" "fstatistic"     "cov.unscaled"

#### Confidence Intervals
confint(satisfaction.fit, parm = c(3, 4), level = 0.95)
              2.5 %    97.5 %
SEVERITY   -1.434831 0.5508228
ANXIETY    -27.797859 0.8575324

#### Hand Computations
X <- as.matrix(cbind(rep(1, nrow(PatSat)), PatSat[2:4]))
b <- solve(t(X) %*% X) %*% t(X) %*% PatSat[[1]]
b
      [,1]
rep(1, nrow(PatSat)) 158.4912517
AGE                 -1.1416118
SEVERITY             -0.4420043
ANXIETY              -13.4701632
dof <- satisfaction.fit$df.residual
dof
[1] 42
qt(0.025, df = dof, lower.tail = F)
[1] 2.018082
```



```
#### Computing Fitted Values
satisfaction.fit$fitted.values[1:2]
      1      2
47.88707 66.07965

yHat <- X %>% b
yHat[1:2]
[1] 47.88707 66.07965

predict(satisfaction.fit)[1:2]
      1      2
47.88707 66.07965

#### Confidence Intervals for Mean Response
nd <- data.frame(AGE = c(37, 38), SEVERITY = c(50, 55), ANXIETY = c(2.8, 2.5))
nd
  AGE SEVERITY ANXIETY
1  37         50     2.8
2  38         55     2.5

predict(satisfaction.fit, newdata = nd, interval = "confidence", level = 0.9)
      fit      lwr      upr
1 56.43494 49.49290 63.37699
2 57.12436 52.92048 61.32824

#### Prediction Intervals
predict(satisfaction.fit, newdata = nd, interval = "prediction", level = 0.99)
      fit      lwr      upr
1 56.43494 27.10185 85.76803
2 57.12436 29.16194 85.08678

nd <- as.matrix(nd[, ])
x.h <- c(1, nd)
y.h <- t(x.h) %>% b
y.h
      [,1]
[1,] 56.43494

#### Mean Square Error
MSE <- satisfaction.summary$sigma^2

#### Variance/Covariance Matrix
vcov(satisfaction.fit)
      (Intercept)      AGE      SEVERITY      ANXIETY
(Intercept) 328.5478428  0.93283693 -6.87207388 -6.8081417
AGE          0.9328369  0.04613853 -0.03223004 -0.4716488
SEVERITY     -6.8720739 -0.03223004  0.24203030 -1.7916031
ANXIETY      -6.8081417 -0.47164876 -1.79160306 50.4051837

MSE * solve(t(X) %>% X)
      rep(1, nrow(PatSat))      AGE      SEVERITY      ANXIETY
rep(1, nrow(PatSat))      328.5478428  0.93283693 -6.87207388 -6.8081417
AGE          0.9328369  0.04613853 -0.03223004 -0.4716488
SEVERITY     -6.8720739 -0.03223004  0.24203030 -1.7916031
ANXIETY      -6.8081417 -0.47164876 -1.79160306 50.4051837
sqrt(MSE * t(x.h) %>% solve(t(X) %>% X) %>% x.h)
      [,1]
[1,] 4.127372

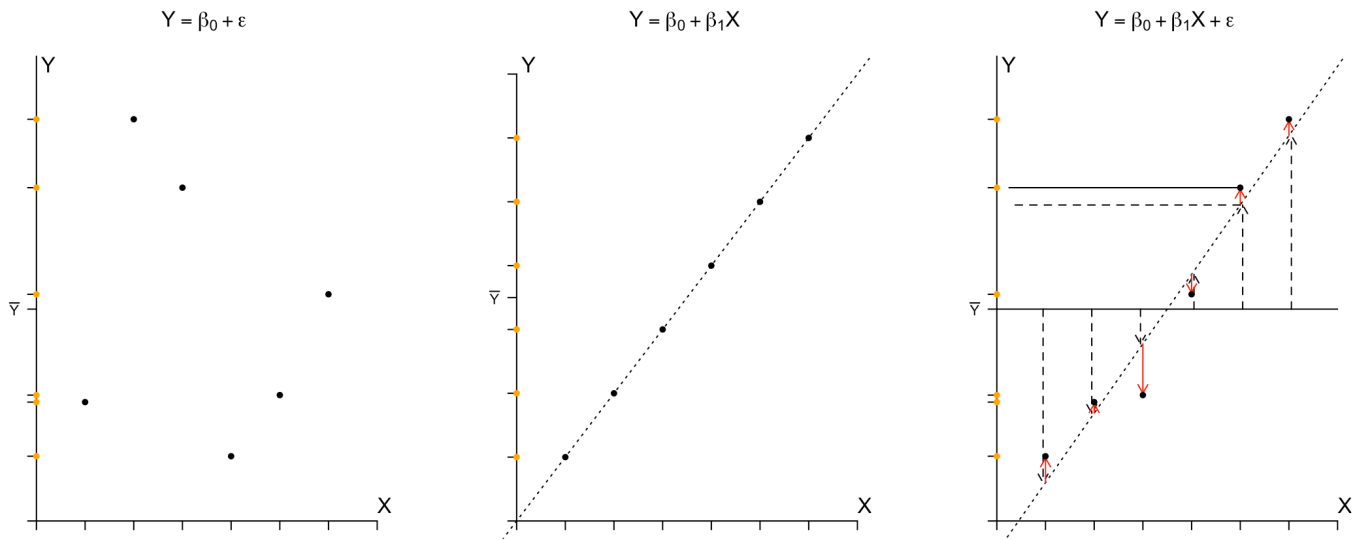
qt(0.95, df = dof, lower.tail = T)
[1] 1.681952

#### Confidence Bands
cv.f <- qf(0.05, df1 = 4, df2 = dof, lower.tail = FALSE)
W <- sqrt(4 * cv.f)
W
[1] 3.221343
```



# Chapter 5: Explaining Variation in Response from its Mean

## Section 1: Partitioning Variation



### Definition:

The  $i^{th}$  deviation of a response value from the overall mean is  $Y_i - \bar{Y}$ .

$$Y_i - \bar{Y} = (Y_i - \hat{Y}_i) + (\hat{Y}_i - \bar{Y})$$

### Note:

- If  $\beta_1 \neq 0$ , then the  $i^{th}$  deviation of the response can be partially explained by the regression relationship between the response and the predictor.
  - This difference is given by  $\hat{Y}_i - \bar{Y}$ .
  - There is a difference between the overall mean of the response **AND** the mean of the response at a particular value of the predictor.
- If  $V(\epsilon > 0)$ , then the deviation of the response can't be entirely explained by the regression relationship.
  - The response varies away from the regression line.
  - This variation is from the random error.
  - It is called **unexplained** variation. Unexplained because the regression relationship can't explain it.

$$\begin{aligned} \sum_{i=1}^n (Y_i - \bar{Y})^2 &= \sum_{i=1}^n (Y_i - \hat{Y}_i)^2 + \sum_{i=1}^n (\hat{Y}_i - \bar{Y})^2 \\ SSTotal &= SSError + SSRegression \\ \text{Total Variation} &= \text{Unexplained Variation} + \text{Explained Variation} \end{aligned}$$

## Section 2: ANOVA TABLE - Simple Linear Regression - Overall F Test

The partitioning of the total variation in the response can be recorded in an ANalysis Of Variance table. Otherwise known as an ANOVA table.

Source	Degrees of Freedom	Sum of Squares	Mean Squares	$F$	Expected(MS)
Regr.	1	$SSReg = \sum(\hat{Y}_i - \bar{Y})^2$	$MSReg = \frac{SSReg}{1}$	$F = \frac{MSReg}{MSE}$	$\sigma^2 + \beta_1^2 \sum(X_i - \bar{X})^2$
Error	$n - 2$	$SSE = \sum(Y_i - \hat{Y}_i)^2$	$MSE = \frac{SSE}{n - 2}$		$\sigma^2$
Total	$n - 1$	$SST = \sum(Y_i - \bar{Y})^2$			

### Degrees of Freedom - A Partition of Information

- $n - 1$  independent pieces of information to be partitioned.
- $n - 2$  of these are used in the Error row.
- 1 is left over for the regression row.

### Expected Mean Squares

$$E(MSReg) = \sigma^2 + \beta_1^2 \sum(X_i - \bar{X})^2 \quad E(MSE) = \sigma^2$$

### Motivation for a test:

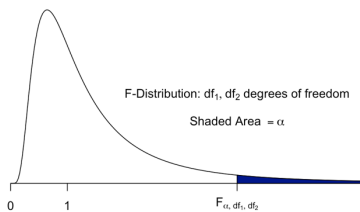
Consider the ration of  $E(MSReg)$  to  $E(MSE)$ .<sup>14</sup> Namely,

$$\frac{E(MSReg)}{E(MSE)} = \begin{cases} \frac{\sigma^2 + \beta_1^2 \sum(X_i - \bar{X})^2}{\sigma^2} & \text{if } \beta_1 \neq 0 \\ \frac{\sigma^2}{\sigma^2} & \text{if } \beta_1 = 0 \end{cases}.$$

## Section 3: F-Test $H_0: \beta_1 = 0$ vs. $H_1: \beta_1 \neq 0$

### Sampling Distribution of $F^*$

For the normal error regression model, if  $\beta_1 = 0$  then  $F^* = \frac{MSReg}{MSE}$  has an  $F$  distribution with 1 numerator degree of freedom and  $n - 2$  denominator degrees of freedom.



<sup>14</sup> Do not misinterpret this to thing that  $E\left(\frac{MSReg}{MSE}\right) = \frac{E(MSReg)}{E(MSE)}$

**Example:**

A materials engineer at a furniture manufacturing site wants to assess the stiffness of the particle board that the manufacturer uses. The engineer collects stiffness data from particle board pieces that have various densities at different temperatures.(Minitab, Mont)

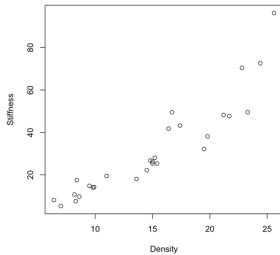
**#### Partial Dataframe**

```
head(PartBoard, n = 3)[1:2]
```

```
  Density Stiffness
1    9.5    14.814
2    8.4    17.502
3    9.8    14.007
```

**#### Plot Data**

```
plot(Stiffness ~ Density, data = PartBoard, xlab = "Density", ylab = "Stiffness")
```

**#### Fitting the Model**

```
particle.fit <- lm(Stiffness ~ Density, data = PartBoard)
```

**#### Summarizing the Fitted Model**

```
summary(particle.fit)
```

Call:

```
lm(formula = Stiffness ~ Density, data = PartBoard)
```

Residuals:

```
      Min       1Q   Median       3Q      Max
-15.3565  -6.6346   0.7408   3.7357  27.1077
```

Coefficients:

```
            Estimate Std. Error t value Pr(>|t|)
(Intercept) -21.5935     4.8647  -4.439 0.000148 ***
Density       3.5465     0.3041  11.662 7.87e-12 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Residual standard error: 9.037 on 26 degrees of freedom

Multiple R-squared: 0.8395, Adjusted R-squared: 0.8333

F-statistic: 136 on 1 and 26 DF, p-value: 7.873e-12

**#### ANOVA TABLE**

```
particle.anova <- anova(particle.fit)
```

```
particle.anova
```

Analysis of Variance Table

Response: Stiffness

```
      Df Sum Sq Mean Sq F value    Pr(>F)
Density  1 11106.5  11106.5   136.01 7.873e-12 ***
Residuals 26  2123.2    81.7
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

**#### Components of ANOVA**

```
names(particle.anova)
```

```
[1] "Df"      "Sum Sq"  "Mean Sq" "F value" "Pr(>F)"
```

```
dof <- particle.anova$Df
```

```
dof
```

```
[1] 1 26
```

**#### Critical Value**

```
qf(0.05, df1 = dof[1], df2 = dof[2], lower.tail = F)
```

```
[1] 4.225201
```

## Section 4: ANOVA TABLE - Multiple Linear Regression - Overall F Test

Source	Degrees of Freedom	Sum of Squares	Mean Squares	$F$	Expected(MS)
Regr.	$p - 1$	$SSReg = \sum(\hat{Y}_i - \bar{Y})^2$	$MSReg = \frac{SSReg}{p - 1}$	$F = \frac{MSReg}{MSE}$	$\sigma^2 + g(\beta_0, \beta_1, \dots, \beta_{p-1})$
Error	$n - p$	$SSE = \sum(Y_i - \hat{Y}_i)^2$	$MSE = \frac{SSE}{n - p}$		$\sigma^2$
Total	$n - 1$	$SST = \sum(Y_i - \bar{Y})^2$			$g(\beta_0, \beta_1, \dots, \beta_{p-1}) \geq 0$

### Degrees of Freedom - A Partition of Information

- $n - 1$  independent pieces of information to be partitioned.
- $n - p$  of these are used in the Error row.
- $p - 1$  is left over for the regression row.

### Expected Mean Squares

$$E(MSReg) = \sigma^2 + \sum[\beta_1(X_{i1} - \bar{X}_1) + \beta_2(X_{i2} - \bar{X}_2) + \dots]^2 = \sigma^2 \quad E(MSE) = \sigma^2$$

### Motivation for a test:

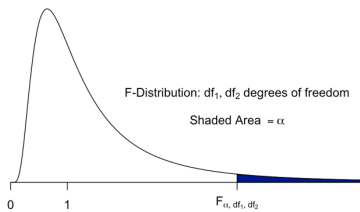
Consider the ration of  $E(MSReg)$  to  $E(MSE)$ .<sup>15</sup> Namely,

$$\frac{E(MSReg)}{E(MSE)} = \begin{cases} \frac{\sigma^2 + g(\beta_0, \beta_1, \dots, \beta_{p-1})}{\sigma^2} & \text{if } \beta_j \neq 0 \text{ for some } j \text{ in } 1, 2, \dots, p - 1 \\ \frac{\sigma^2}{\sigma^2} & \text{otherwise} \end{cases}.$$

## Section 5: F-Test $H_0: \beta_1 = \beta_2 = \dots = \beta_{p-1} = 0$ vs. $H_1$ : At least one $\beta_i \neq 0$

### Sampling Distribution of $F^*$

For the normal error regression model, if  $\beta_1 = \beta_2 = \dots = \beta_{p-1} = 0$  then  $F^* = \frac{MSReg}{MSE}$  has an  $F$  distribution with  $p - 1$  numerator degree of freedom and  $n - p$  denominator degrees of freedom.



<sup>15</sup> Do not misinterpret this to thing that  $E\left(\frac{MSReg}{MSE}\right) = \frac{E(MSReg)}{E(MSE)}$

**Example:**

A hospital administrator wished to study the relationship between patient satisfaction  $Y$  and patient's age  $X_1$ , severity of illness  $X_2$ , and anxiety level  $X_3$ . The administrator randomly selected 46 patients. The data is held in the PatSat dataset. Larger values for  $Y$ ,  $X_2$  and  $X_3$  indicate higher satisfaction, severity and anxiety.(K)

```
#### Fitting the Model
satisfaction.fit <- lm(SAT ~ AGE + SEVERITY + ANXIETY, data = PatSat)

#### Components of the Fitted Model
names(satisfaction.fit)
[1] "coefficients" "residuals"      "effects"      "rank"
[5] "fitted.values" "assign"         "qr"           "df.residual"
[9] "xlevels"      "call"          "terms"        "model"

#### Summarizing the Fitted Model
satisfaction.summary <- summary(satisfaction.fit)
satisfaction.summary

Call:
lm(formula = SAT ~ AGE + SEVERITY + ANXIETY, data = PatSat)

Residuals:
    Min       1Q   Median       3Q      Max
-18.3524  -6.4230   0.5196   8.3715  17.1601

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  158.4913    18.1259   8.744 5.26e-11 ***
AGE          -1.1416     0.2148  -5.315 3.81e-06 ***
SEVERITY     -0.4420     0.4920  -0.898  0.3741
ANXIETY     -13.4702     7.0997  -1.897  0.0647 .
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 10.06 on 42 degrees of freedom
Multiple R-squared:  0.6822,    Adjusted R-squared:  0.6595
F-statistic: 30.05 on 3 and 42 DF,  p-value: 1.542e-10

names(satisfaction.summary)
[1] "call"      "terms"      "residuals"  "coefficients"
[5] "aliased"   "sigma"      "df"         "r.squared"
[9] "adj.r.squared" "fstatistic" "cov.unscaled"

#### SEQUENTIAL ANOVA TABLE
satisfaction.anova <- anova(satisfaction.fit)
satisfaction.anova
Analysis of Variance Table

Response: SAT
      Df Sum Sq Mean Sq F value    Pr(>F)
AGE     1  8275.4   8275.4  81.8026 2.059e-11 ***
SEVERITY 1   480.9    480.9   4.7539  0.03489 *
ANXIETY  1   364.2    364.2   3.5997  0.06468 .
Residuals 42 4248.8    101.2
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
#### NOT THE ANOVA TABLE WE WANT DOES NOT INCLUDE OVERALL F TEST
```

## Section 6: General Linear Test

This approach to testing allows you to include some predictors and test whether others should be included in the model.

### Definition:

A **full** or **unrestricted** model is a model that includes all predictors of possible interest.

### Definition:

The **reduced** or **restricted** model is a version of the full model with pre-specified parameters set to zero.<sup>16</sup>

$$\begin{array}{c}
 \text{Full Model} \\
 \hline
 \text{Reduced Model} \\
 \hline
 Y \sim X_1 + X_2 + \cdots + X_r + X_{r+1} + X_{r+2} + \cdots + X_{r+t}
 \end{array}$$

$$\begin{array}{ll}
 \text{Full Model:} & Y_i = \beta_0 + \beta_1 X_{i,1} + \beta_2 X_{i,2} + \cdots + \beta_r X_{i,r} + \beta_{r+1} X_{i,r+1} + \cdots + \beta_{r+t} X_{i,r+t} + \epsilon_i \\
 \text{Reduced Model:} & Y_i = \beta_0 + \beta_1 X_{i,1} + \beta_2 X_{i,2} + \cdots + \beta_r X_{i,r} + \epsilon_i
 \end{array}$$

### Hypotheses:

$$\begin{array}{ll}
 H_0: & \beta_{r+1} = \beta_{r+2} = \cdots = \beta_{r+t} = 0 \quad (\text{Reduced Model}) \\
 H_1: & \text{at least one of } \beta_{r+1}, \dots, \beta_{r+t} \neq 0 \quad (\text{Full Model})
 \end{array}$$

$$\begin{array}{c}
 \text{Alternative Hypothesis} \\
 \text{At least one of } \beta_{r+1}, \dots, \beta_{r+t} \neq 0 \\
 \hline
 \text{Null Hypothesis} \\
 \beta_{r+1} = \cdots = \beta_{r+t} = 0 \\
 \hline
 Y \sim X_1 + X_2 + \cdots + X_r + X_{r+1} + X_{r+2} + \cdots + X_{r+t}
 \end{array}$$

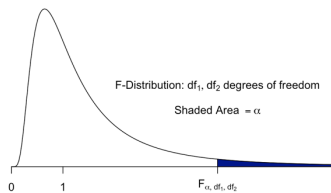
### Least Squares

$$\min \text{SS}(b_0^*, b_1^*, \dots, b_r^*, b_{r+1}, \dots, b_{r+t}) = \text{SSE}(\text{Full}) \leq \text{SSE}(\text{Reduced}) = \min \text{SS}(b_0^*, b_1^*, \dots, b_r^*, 0, \dots, 0)$$

### Test Statistic:

Assuming the assumptions for the normal error multiple linear regression model are satisfied, the test statistic  $F$  for the General Linear Test will have an  $F$  distribution with  $df_1 = DF_{\text{Reduce}} - DF_{\text{FULL}}$  and  $df_2 = DF_{\text{FULL}}$ . The test statistic is given by

$$F = \frac{\left( \frac{\text{SSE}(\text{Reduced}) - \text{SSE}(\text{Full})}{df_{\text{Reduced}} - df_{\text{Full}}} \right)}{\left( \frac{\text{SSE}(\text{Full})}{df_{\text{Full}}} \right)}$$



- $\text{SSE}(\text{Full})$  = Amount of Variation NOT explained by FULL Model
- $\text{SSE}(\text{Reduced}) - \text{SSE}(\text{Full}) = \text{SSREG}(\text{Full}) - \text{SSREG}(\text{Reduced}) =$   
Amount of variation explained by full model but NOT by the reduced model

<sup>16</sup> The most reduced model you can have does not use any predictor variables. The model is built only on the intercept. It is commonly written as  $Y \sim 1$ .



### Simple Linear Regression Example:

A materials engineer at a furniture manufacturing site wants to assess the stiffness of the particle board that the manufacturer uses. The engineer collects stiffness data from particle board pieces that have various densities at different temperatures. (Minitab, Mont)

```
#### Partial Dataframe
head(PartBoard)
  Density Stiffness    Temp
1    9.5    14.814 70.61056
2    8.4    17.502 73.34893
3    9.8    14.007 66.15377
4   11.0    19.443 70.05781
5    8.3    7.573 69.33919
6    9.9    14.191 69.12882

#### Fitting Full Model
particle.fit <- lm(Stiffness ~ Density, data = PartBoard)

#### Fitting Reduced Model
particle.intercept.only <- lm(Stiffness ~ 1, data = PartBoard)
```

```
#### Summarizing Full Model
summary(particle.fit)

Call:
lm(formula = Stiffness ~ Density, data = PartBoard)

Residuals:
    Min       1Q   Median       3Q      Max
-15.3565  -6.6346   0.7408   3.7357  27.1077

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) -21.5935     4.8647  -4.439 0.000148 ***
Density       3.5465     0.3041  11.662 7.87e-12 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 9.037 on 26 degrees of freedom
Multiple R-squared:  0.8395,    Adjusted R-squared:  0.8333
F-statistic: 136 on 1 and 26 DF, p-value: 7.873e-12
```

```
#### ANOVA TABLE - OVERALL F-TEST:
particle.anova <- anova(particle.fit)
particle.anova
Analysis of Variance Table

Response: Stiffness
      Df Sum Sq Mean Sq F value    Pr(>F)
Density  1 11106.5 11106.5  136.01 7.873e-12 ***
Residuals 26  2123.2    81.7
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```
#### GENERAL LINEAR TEST
anova(particle.intercept.only, particle.fit)
Analysis of Variance Table

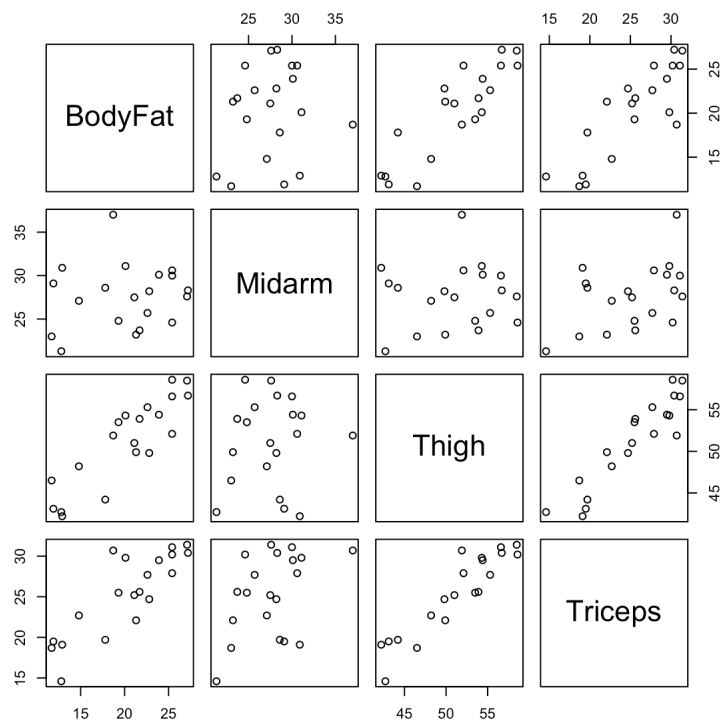
Model 1: Stiffness ~ 1
Model 2: Stiffness ~ Density
      Res.Df  RSS Df Sum of Sq    F    Pr(>F)
1         27 13229.7
2         26 2123.2  1    11106 136.01 7.873e-12 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Example:

A researcher is exploring the relationship between body fat (Y) and three predictors: Tricep Skinfold Thickness, Thigh Circumference, and Midarm Circumference.(Kutner)

```
#### Partial Dataframe
head(BodyFat)
  BodyFat Midarm Thigh Triceps
1   11.9   29.1  43.1   19.5
2   22.8   28.2  49.8   24.7
3   18.7   37.0  51.9   30.7
4   20.1   31.1  54.3   29.8
5   12.9   30.9  42.2   19.1
6   21.7   23.7  53.9   25.6

#### Scatterplot Matrix
pairs(BodyFat)
```



```
#### Correlation Matrix
cor(BodyFat)
  BodyFat  Midarm  Thigh  Triceps
BodyFat 1.000000 0.142444 0.878089 0.843265
Midarm  0.142444 1.000000 0.084667 0.457772
Thigh    0.878089 0.084667 1.000000 0.923842
Triceps  0.843265 0.457772 0.923842 1.000000
```

## Overall F Test - Multiple Linear Regression

### Recall:

The overall F test is used for the following hypotheses:

$$H_0: \beta_1 = \beta_2 = \dots = \beta_{p-1} = 0 \quad Y \sim 1 \quad (\text{Reduced Model})$$

$$H_1: \text{at least one of } \beta_1, \dots, \beta_{p-1} \neq 0 \quad Y \sim X_1 + X_2 + \dots + X_{p-1} \quad (\text{Full Model})$$

#### #### Fitting Full Model

```
body.fit.all <- lm(BodyFat ~ Midarm + Thigh + Triceps, data = BodyFat)
```

#### #### Summarizing Full Model

```
summary(body.fit.all)
```

Call:

```
lm(formula = BodyFat ~ Midarm + Thigh + Triceps, data = BodyFat)
```

Residuals:

	Min	1Q	Median	3Q	Max
	-3.7263	-1.6111	0.3923	1.4656	4.1277

Coefficients:

	Estimate	Std. Error	t value	Pr(> t )
(Intercept)	117.085	99.782	1.173	0.258
Midarm	-2.186	1.595	-1.370	0.190
Thigh	-2.857	2.582	-1.106	0.285
Triceps	4.334	3.016	1.437	0.170

Residual standard error: 2.48 on 16 degrees of freedom

Multiple R-squared: 0.8014, Adjusted R-squared: 0.7641

F-statistic: 21.52 on 3 and 16 DF, p-value: 7.343e-06

#### #### SEQUENTIAL ANOVA TABLE FULL MODEL

```
body.all.anova <- anova(body.fit.all)
```

```
body.all.anova
```

Analysis of Variance Table

Response: BodyFat

	Df	Sum Sq	Mean Sq	F value	Pr(>F)
Midarm	1	10.05	10.05	1.6343	0.2193
Thigh	1	374.23	374.23	60.8471	7.684e-07 ***
Triceps	1	12.70	12.70	2.0657	0.1699
Residuals	16	98.40	6.15		

---

Signif. codes: 0 '\*\*\*' 0.001 '\*\*' 0.01 '\*' 0.05 '.' 0.1 ' ' 1

	Source	DF	SS	MS	F	P-value
	Model	3	397	132	22	7.343e - 06
	Error	16	98	6.2		
	Total	19	495			

#### #### Fitting Full Model & Intercept Only Model

```
body.fit.all <- lm(BodyFat ~ Midarm + Thigh + Triceps, data = BodyFat)
```

```
body.intercept.only <- lm(BodyFat ~ 1, data = BodyFat)
```

#### #### Summarizing Full Model

```
anova(body.intercept.only, body.fit.all)
```

Analysis of Variance Table

Model 1: BodyFat ~ 1

Model 2: BodyFat ~ Midarm + Thigh + Triceps

	Res.Df	RSS	Df	Sum of Sq	F	Pr(>F)
1	19	495.39				
2	16	98.40	3	396.98	21.516	7.343e-06 ***

---

Signif. codes: 0 '\*\*\*' 0.001 '\*\*' 0.01 '\*' 0.05 '.' 0.1 ' ' 1

## General Linear Tests - Multiple Linear Regression

### Example:

A researcher is exploring the relationship between body fat (Y) and three predictors: Tricep Skinfold Thickness, Thigh Circumference, and Midarm Circumference.(Kutner)

```
#### Fitting Full Model & Midarm Only Model
body.fit.all <- lm(BodyFat ~ Midarm + Thigh + Triceps, data = BodyFat)
body.midarm.only <- lm(BodyFat ~ Midarm, data = BodyFat)
```

```
#### Summarizing Full Model
summary(body.fit.all)
```

```
Call:
lm(formula = BodyFat ~ Midarm + Thigh + Triceps, data = BodyFat)
```

```
Residuals:
    Min       1Q   Median       3Q      Max
-3.7263 -1.6111  0.3923  1.4656  4.1277
```

```
Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  117.085     99.782   1.173   0.258
Midarm        -2.186      1.595  -1.370   0.190
Thigh         -2.857      2.582  -1.106   0.285
Triceps        4.334      3.016   1.437   0.170
```

```
Residual standard error: 2.48 on 16 degrees of freedom
Multiple R-squared:  0.8014,    Adjusted R-squared:  0.7641
F-statistic: 21.52 on 3 and 16 DF,  p-value: 7.343e-06
```

Midarm:	$H_0$ :	BodyFat ~ Thigh + Tricep	$H_a$ :	BodyFat ~ Thigh + Tricep + Midarm
Thigh:	$H_0$ :	BodyFat ~ Tricep + Midarm	$H_a$ :	BodyFat ~ Tricep + Midarm + Thigh
Triceps:	$H_0$ :	BodyFat ~ Thigh + Midarm	$H_a$ :	BodyFat ~ Thigh + Midarm + Tricep
F:	$H_0$ :	BodyFat ~ 1	$H_a$ :	BodyFat ~ Thigh + Tricep + Midarm

### #### SEQUENTIAL ANOVA TABLE FULL MODEL

```
anova(body.fit.all)
Analysis of Variance Table

Response: BodyFat
      Df Sum Sq Mean Sq F value    Pr(>F)
Midarm  1  10.05   10.05  1.6343    0.2193
Thigh   1 374.23  374.23 60.8471 7.684e-07 ***
Triceps 1  12.70   12.70  2.0657    0.1699
Residuals 16  98.40    6.15
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Midarm:	$H_0$ :	BodyFat ~ 1	$H_a$ :	BodyFat ~ Midarm
Thigh:	$H_0$ :	BodyFat ~ Midarm	$H_a$ :	BodyFat ~ Midarm + Thigh
Triceps:	$H_0$ :	BodyFat ~ Midarm + Thigh + Midarm	$H_a$ :	BodyFat ~ Midarm + Thigh + Tricep

### #### Summarizing Full Model - Midarm only vs ALL

```
anova(body.midarm.only, body.fit.all)
Analysis of Variance Table

Model 1: BodyFat ~ Midarm
Model 2: BodyFat ~ Midarm + Thigh + Triceps
      Res.Df  RSS Df Sum of Sq    F    Pr(>F)
1         18 485.34
2         16  98.40  2    386.93 31.456 2.856e-06 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

#### #### Fitting Full Model - Order of Predictors Reversed

```
body.fit.rev <- lm(BodyFat ~ Triceps + Thigh + Midarm, data = BodyFat)
```

#### #### ANOVA Table - Order of Predictors Reversed

```
anova(body.fit.rev)
```

Analysis of Variance Table

Response: BodyFat

	Df	Sum Sq	Mean Sq	F value	Pr(>F)
Triceps	1	352.27	352.27	57.2768	1.131e-06 ***
Thigh	1	33.17	33.17	5.3931	0.03373 *
Midarm	1	11.55	11.55	1.8773	0.18956
Residuals	16	98.40	6.15		

---

Signif. codes: 0 '\*\*\*' 0.001 '\*\*' 0.01 '\*' 0.05 '.' 0.1 ' ' 1

#### #### ANOVA Table - Original Order of Predictors

```
anova(body.fit.all)
```

Analysis of Variance Table

Response: BodyFat

	Df	Sum Sq	Mean Sq	F value	Pr(>F)
Midarm	1	10.05	10.05	1.6343	0.2193
Thigh	1	374.23	374.23	60.8471	7.684e-07 ***
Triceps	1	12.70	12.70	2.0657	0.1699
Residuals	16	98.40	6.15		

---

Signif. codes: 0 '\*\*\*' 0.001 '\*\*' 0.01 '\*' 0.05 '.' 0.1 ' ' 1

#### #### Summarizing Full Model - Order of Predictors Reversed

```
summary(body.fit.rev)
```

Call:

```
lm(formula = BodyFat ~ Triceps + Thigh + Midarm, data = BodyFat)
```

Residuals:

	Min	1Q	Median	3Q	Max
	-3.7263	-1.6111	0.3923	1.4656	4.1277

Coefficients:

	Estimate	Std. Error	t value	Pr(> t )
(Intercept)	117.085	99.782	1.173	0.258
Triceps	4.334	3.016	1.437	0.170
Thigh	-2.857	2.582	-1.106	0.285
Midarm	-2.186	1.595	-1.370	0.190

Residual standard error: 2.48 on 16 degrees of freedom

Multiple R-squared: 0.8014, Adjusted R-squared: 0.7641

F-statistic: 21.52 on 3 and 16 DF, p-value: 7.343e-06

#### #### Summarizing Full Model - Original Order of Predictors

```
summary(body.fit.all)
```

Call:

```
lm(formula = BodyFat ~ Midarm + Thigh + Triceps, data = BodyFat)
```

Residuals:

	Min	1Q	Median	3Q	Max
	-3.7263	-1.6111	0.3923	1.4656	4.1277

Coefficients:

	Estimate	Std. Error	t value	Pr(> t )
(Intercept)	117.085	99.782	1.173	0.258
Midarm	-2.186	1.595	-1.370	0.190
Thigh	-2.857	2.582	-1.106	0.285
Triceps	4.334	3.016	1.437	0.170

Residual standard error: 2.48 on 16 degrees of freedom

Multiple R-squared: 0.8014, Adjusted R-squared: 0.7641

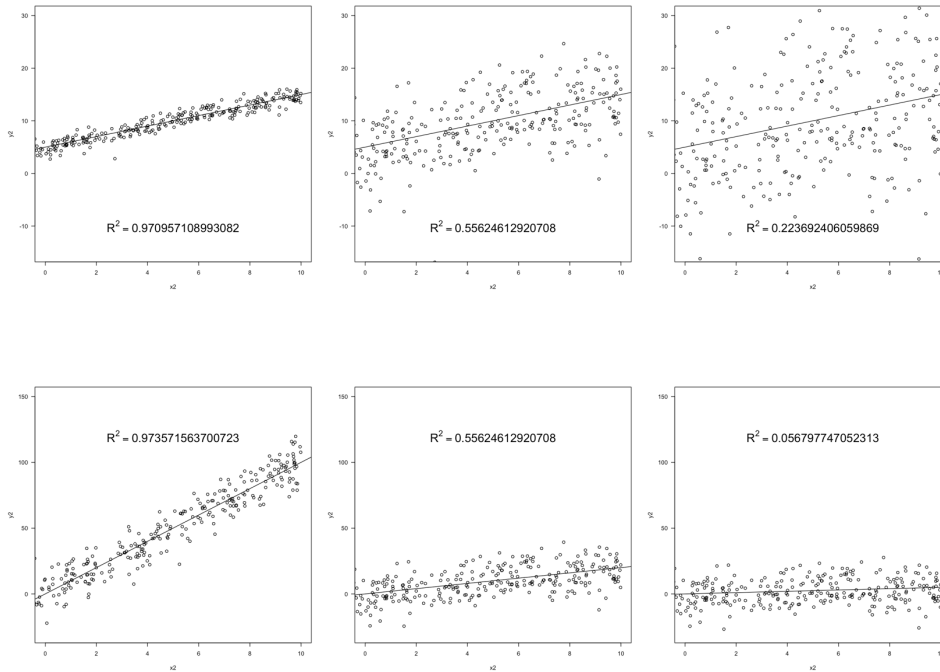
F-statistic: 21.52 on 3 and 16 DF, p-value: 7.343e-06

## Section 7: Coefficient Of Determination

### Definition:

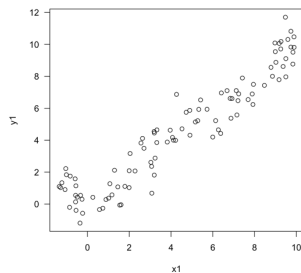
The **coefficient of determination**  $R^2$  is the proportion of deviation/variance explained by regression.

$$R^2 = \frac{SS_{Reg}}{SST} = 1 - \frac{SSE}{SST}$$



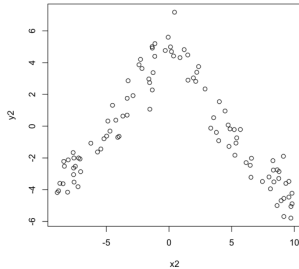
**A high  $R^2$  value doesn't necessarily indicate that regression line is a good fit.**

```
par(las = 1)
set.seed(6)
n <- 100
x1 <- runif(n, min = -2, max = 10)
y1 <- abs(x1) + rnorm(n, sd = 1)
summary(lm(y1 ~ x1))$r.squared
[1] 0.8930766
plot(x1, y1)
```



**An  $R^2$  value near zero doesn't necessarily indicate that the variables are not related.**

```
set.seed(6)
x2 <- runif(n, min = -10, max = 10)
y2 <- -abs(x2) + rnorm(n, sd = 1) + 5
summary(lm(y2 ~ x2))$r.squared
[1] 0.03905343
plot(x2, y2)
```



**As the number of explanatory variables increases,  $R^2$  increases, even if they are meaningless variables.**

**Example:**

A hospital administrator wished to study the relationship between patient satisfaction  $Y$  and patient's age  $X_1$ , severity of illness  $X_2$ , and anxiety level  $X_3$ . The administrator randomly selected 46 patients. The data is held in the PatSat dataset. Larger values for  $Y$ ,  $X_2$  and  $X_3$  indicate higher satisfaction, severity and anxiety. (K)

```
#### Fitting SAT ~ AGE
satisfaction.fit1 <- lm(SAT ~ AGE, data = PatSat)

summary(satisfaction.fit1)$r.squared  #### R-Squared
[1] 0.6189843

#### Fitting SAT ~ AGE + SEVERITY
satisfaction.fit2 <- lm(SAT ~ AGE + SEVERITY, data = PatSat)
summary(satisfaction.fit2)$r.squared  #### R-Squared
[1] 0.6549559

#### Fitting SAT ~ AGE + SEVERITY + ANXIETY
satisfaction.fit.all <- lm(SAT ~ AGE + SEVERITY + ANXIETY, data = PatSat)
summary(satisfaction.fit.all)$r.squared  #### R-Squared
[1] 0.6821943

#### Generating Junk Variable
junk.Variable <- rnorm(nrow(PatSat), sd = 10)

#### Fitting SAT ~ AGE + SEVERITY + ANXIETY +junk.Variable
satisfaction.fit.junk <- lm(SAT ~ AGE + SEVERITY + ANXIETY + junk.Variable, data = PatSat)
summary(satisfaction.fit.junk)

Call:
lm(formula = SAT ~ AGE + SEVERITY + ANXIETY + junk.Variable,
    data = PatSat)

Residuals:
    Min       1Q   Median       3Q      Max
-16.4690  -5.9766   0.3852   9.1106  15.3285

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  158.0685    18.0311   8.766 6.03e-11 ***
AGE          -1.1949     0.2181  -5.478 2.39e-06 ***
SEVERITY     -0.3912     0.4911  -0.797  0.4303
ANXIETY     -13.4459     7.0612  -1.904  0.0639 .
junk.Variable  0.1917     0.1587   1.208  0.2341
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 10 on 41 degrees of freedom
Multiple R-squared:  0.6931,    Adjusted R-squared:  0.6632
F-statistic: 23.15 on 4 and 41 DF,  p-value: 4.626e-10
```

## Section 8: Multiple Inference

### Which Test? Which Variables?

1. Overall F Test  $H_0: \beta_1 = \beta_2 = \dots = \beta_{p-1} = 0$

$$X_1, X_2, \dots, X_{p-1}$$

2. Tests on Subsets:  $H_0: \beta_{r+1} = \beta_{r+2} = \dots = \beta_{r+t}$

$$X_1, X_2, \dots, X_r$$

$$X_{r+1}, X_{r+2}, \dots, X_{r+t}$$

### Bonferroni Inequality

Suppose that  $A_1, A_2, \dots, A_k$  are events. Using the Addition Rule, we have the following inequalities:

$$P(A_1 \text{ or } A_2) = P(A_1) + P(A_2) - P(A_1 \text{ and } A_2) \leq P(A_1) + P(A_2)$$

$$P(A_1 \text{ or } A_2 \text{ or } A_3) = P([A_1 \text{ or } A_2] \text{ or } A_3)$$

$$P(A_1 \text{ or } A_2 \text{ or } \dots \text{ or } A_k) \leq P(A_1) + P(A_2) + \dots + P(A_k)$$

### Multiple Tests

#### **Definition:**

Suppose you are performing  $k$  hypothesis tests. Define the event  $A_i$  = Type I error on the  $i^{th}$  test,  $i = 1, 2, \dots, k$ . Further, let  $\alpha_i$  = significance level of the  $i^{th}$  test. Then **overall/experiment-wise error rate** on  $k$  simultaneous hypothesis tests is  $\alpha_e = P(\text{at least one Type I error in } k \text{ tests})$ .

#### **Upper Bound:**

An upper bound can be found on the experiment-wise error rate,  $\alpha_e$ , using the inequalities given above.

$$\begin{aligned} P(A_1 \text{ or } A_2 \text{ or } \dots \text{ or } A_k) &\leq P(A_1) + P(A_2) + \dots + P(A_k) \\ &= \alpha_1 + \alpha_2 + \dots + \alpha_k \end{aligned}$$

To control the experiment-wise error rate:

- a. Select a value  $\alpha_{max}$  that represents the maximum experiment-wise error rate that you will allow.
- b. Select  $\alpha_1, \alpha_2, \dots, \alpha_k$  for each test so that  $\alpha_1 + \alpha_2 + \dots + \alpha_k \leq \alpha_{max}$ .

Then the actual experiment-wise error rate  $\alpha_e \leq \alpha_1 + \alpha_2 + \dots + \alpha_k \leq \alpha_{max}$ .

#### **Example:**

Suppose  $\alpha_{max} = 0.05$  and  $k = 10$ . Assuming you will use equal Type I error rates on each test. What should be the Type I error rates on each test?



## Multiple Confidence Intervals

### **Definition:**

Suppose you are to construct  $k$  confidence intervals. Define the event  $A_i = i^{th}$  confidence interval misses its target,  $i = 1, 2, \dots, k$ . Further, let  $\alpha_i =$  significance level of corresponding to the  $i^{th}$  confidence interval. Then the **simultaneous confidence level**  $CL_{all}\%$  on the  $k$  confidence intervals is  $100 \times (1 - \alpha_e)\%$  where  $(1 - \alpha_e) = P(\text{all } k \text{ confidence intervals are correct})$ .

### **Lower Bound:**

An lower bound can be found on the simultaneous confidence level,  $CL_{all}\%$ , using the inequalities given on the previous page.

$$\begin{aligned}
 CL_{all}/100 &= P(\text{all } k \text{ confidence intervals are correct}) \\
 &= 1 - P(\text{at least one CI misses its target}) \\
 &= 1 - P(A_1 \text{ or } A_2 \text{ or } \dots \text{ or } A_k) \\
 &\geq 1 - (P(A_1) + P(A_2) + \dots + P(A_k)) \\
 &= 1 - (\alpha_1 + \alpha_2 + \dots + \alpha_k)
 \end{aligned}$$

To control the simultaneous confidence level:

- select a value  $CL_{min}\%$  that represents the minimum simultaneous confidence level that you will allow.
- Determine the corresponding value  $\alpha_{max}$  where  $1 - \alpha_{max} = CL_{min}/100$ .
- Set the confidence level for each individual confidence interval to  $100(1 - \alpha_1)\%$ ,  $100(1 - \alpha_2)\%$ , ...,  $100(1 - \alpha_k)\%$  so that  $\alpha_1 + \alpha_2 + \dots + \alpha_k \leq \alpha_{max}$ .

Then the actual simultaneous confidence level is

$$CL_{all} \geq 100 \times (1 - (\alpha_1 + \alpha_2 + \dots + \alpha_k)) \geq CL_{min}$$

### **Example:**

Suppose  $CL_{min} = 95\%$  and  $k = 10$ . Assuming you will use equal individual confidence levels for each confidence intervals. What should be the confidence level be for each confidence interval?



