# 1. Simple Linear Regression

- **Regression** used to study the relationship between quantitative variables (e.g. height and weight)
- Collect data on two or more variables
- Two variables simple linear regression (Chapter 1)
- More than two variables **multiple regression** (Chapter 2)
- Response variable (Y) = variable to be predicted
- Predictor variable (X) = variable used to predict Y
- $(x_i,y_i)$  = observed values of X and Y for  $i^{th}$  case.
- Number of cases = n

Height (X)	Weight (Y)
X1	<b>y</b> 1
X2	<b>y</b> <sub>2</sub>
	·
	·
	·
X <sub>n</sub>	y <sub>n</sub>

#### **Outline of simple linear regression**

- Assume there is a linear relationship between X and Y:  $Y = \beta_0 + \beta_1 X$
- $\beta_0$  is the intercept (value of Y when X = 0) and  $\beta_1$  is the slope (change in Y for a unit change in X)
- Estimate  $\beta_0$  and  $\beta_1$  from the data
- Use model to predict Y for given X

#### Methods of linear regression

- Draw scatter plot of points  $(x_i, y_i)$ ; does relationship look approximately linear?
- If so, find the **line of closest fit** to the points; estimate  $\beta_0$  and  $\beta_1$  from the data
- How well does the model fit? Any outliers?
- Would other models give better fit?

$$Y = \beta_0 + \beta_1 X + \beta_2 X^2$$
 (Quadratic in X)?

$$Y = \beta_0 + \beta_1 X + \beta_2 Z$$
, where  $Z = Age$  (Multiple regression)?

#### **Forbes Data Set**

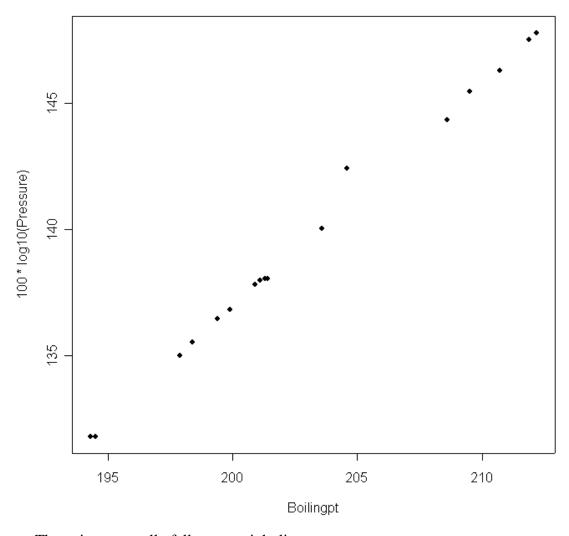
- Atmospheric pressure (measured by mercury barometer) determines altitude
- Low pressure corresponds to high altitude & high pressure corresponds to low altitude
- Use boiling point of water as alternative to measuring atmospheric pressure.
- As atmospheric pressure ↑, boiling point of water ↑ (e.g. pressure cooker)
- As atmospheric pressure  $\downarrow$ , boiling point of water  $\downarrow$
- Use boiling point of water to predict pressure
- Forbes(1857) measured boiling point of water and pressure at 17 locations
- Theory suggests a model of the form

$$Y = \beta_0 + \beta_1 \, X$$
 where  $Y = 100 \, log(Pressure)$ , and Pressure is measured in inches of mercury (Hg) and  $X = Boiling$  point of water in  ${}^{\circ}F$ 

Case	Boiling Pt (°F)	Pressure (in Hg)	Log(Pressure)	100xLog(Pressure)
1	194.5	20.79	1.3179	131.79
2	194.3	20.79	1.3179	131.79
3	197.9	22.40	1.3502	135.02
4	198.4	22.67	1.3555	135.55
5	199.4	23.15	1.3646	136.46
6	199.9	23.35	1.3683	136.83
7	200.9	23.89	1.3782	137.82
8	201.1	23.99	1.3800	138.00
9	201.4	24.02	1.3806	138.06
10	201.3	24.01	1.3804	138.04
11	203.6	25.14	1.4004	140.04
12	204.6	26.57	1.4244	142.44
13	209.5	28.49	1.4547	145.47
14	208.6	27.76	1.4434	144.34
15	210.7	29.04	1.4630	146.30
16	211.9	29.88	1.4754	147.54
17	212.2	30.06	1.4780	147.80

## **Scatter plot for Forbes data**

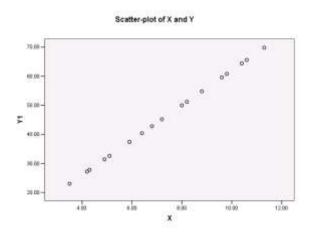
# Plot of 100\*log10(Pressure) vs. Boiling Point

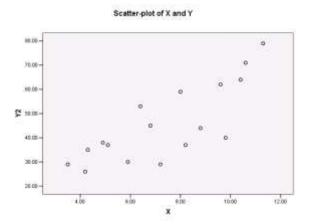


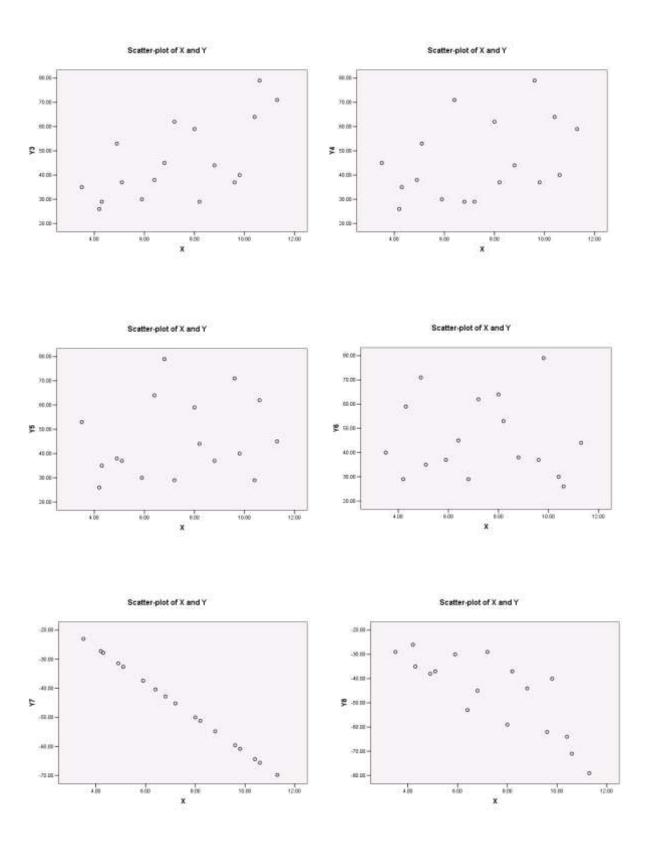
- The points generally fall on a straight line
- There is one "outlier"

# Examples of Scatter plots:

X	Y1	Y2	Y3	Y4	Y5	Y6	Y7	Y8
3.5	23.0	29	35	45	53	40	-23.0	-29
4.2	27.2	26	26	26	26	29	-27.2	-26
4.3	27.8	35	29	35	35	59	-27.8	-35
4.9	31.4	38	53	38	38	71	-31.4	-38
5.1	32.6	37	37	53	37	35	-32.6	-37
5.9	37.4	30	30	30	30	37	-37.4	-30
6.4	40.4	53	38	71	64	45	-40.4	-53
6.8	42.8	45	45	29	79	29	-42.8	-45
7.2	45.2	29	62	29	29	62	-45.2	-29
8.0	50.0	59	59	62	59	64	-50.0	-59
8.2	51.2	37	29	37	44	53	-51.2	-37
8.8	54.8	44	44	44	37	38	-54.8	-44
9.6	59.6	62	37	79	71	37	-59.6	-62
9.8	60.8	40	40	37	40	79	-60.8	-40
10.4	64.4	64	64	64	29	30	-64.4	-64
10.6	65.6	71	79	40	62	26	-65.6	-71
11.3	69.8	79	71	59	45	44	-69.8	-79







## **Assumptions about errors**

Real data will almost never fall exactly on a straight line. For most (or all) points there will be an error. These errors could be

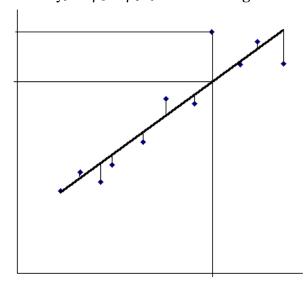
- Measurement errors impossible to measure continuous variables completely accurately.
- The effect of variables not included in the model.
- Natural variability.

We incorporate these errors into the **simple linear regression model** as follows:

$$y_i \ = \ \beta_0 \ + \beta_1 \, x_i + e_i \ , \ \text{where} \ e_i = \text{error} \ \text{for the} \ i^{th} \ \text{case}$$
 and

and

 $y_i = \beta_0 + \beta_1 x_i$  is the **true regression line** of Y on X



We make **assumptions** about errors e<sub>i</sub>:

- needed to prove the optimality of the estimates for  $\beta_0$  and  $\beta_1$
- needed to find confidence intervals for  $\beta_0$  and  $\beta_1$
- tests for these assumptions in Chapter 3/4 (**regression diagnostics**)

## $e_i \sim NID(0, \sigma^2)$

- e<sub>i</sub> are **Normally** distributed with mean 0
- $e_i$  have **common variance**  $\sigma^2$
- e<sub>i</sub> are **independent** variables

Assumptions about e<sub>i</sub> can be expressed in terms of covariance

$$E(e_i) = 0$$
,  $var(e_i) = \sigma^2$ ,  $cov(e_i,e_i) = 0$ , for  $i \neq j$ 

With the normality assumption, this implies that the e<sub>i</sub>'s are independent

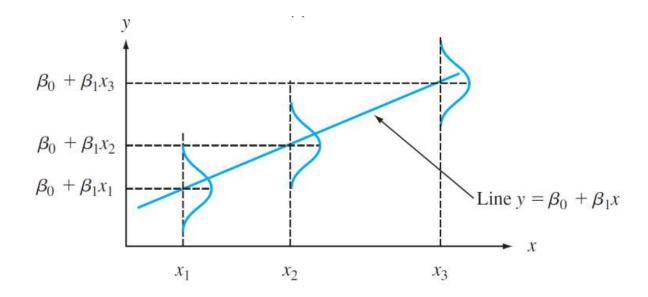
When applying a regression model, these assumptions have to be verified.

## Visualizing the assumptions:

In the simple linear model  $(y_i = \beta_0 + \beta_1 x_i + e_i, e_i \sim \text{NID}(0, \sigma^2))$  we consider the values  $x_i$  as known **constants.** 

i.e. we set  $X = x_i$  and observe the response  $y_i$ . Hence  $var(y_i) = var(\beta_0 + \beta_1 x_i + e_i) = var(\beta_0) + var(\beta_1 x_i) + var(e_i) = 0 + 0 + var(e_i) = \sigma^2$ .

We can visualize the Normality and equal variance assumptions as follows:



#### **Covariance and independent variables**

A and B are **independent events** if P(A|B) = P(A)

i.e., knowing that B has occurred doesn't affect the probability of A Equivalently, A and B are independent events if P(A and B) = P(A)P(B)

X and Y are **independent discrete variables** if

$$P(X = x \text{ and } Y = y) = P(X = x)P(Y = y)$$

X and Y are independent continuous variables if

joint pdf of X and Y =  $h(x,y) = f_X(x) g_Y(y)$  - the product of individual pdfs

Covariance of X and Y =  $cov(X,Y) = E(X - \mu_1)(Y - \mu_2)$ , where  $\mu_1 = E(X)$  and  $\mu_2 = E(Y)$ 

If X and Y are **independent**, then cov(X,Y) = 0:

$$cov(X,Y) = E(X - \mu_1)(Y - \mu_2) = \int (x - \mu_1) f_X(x) dx \bullet \int (y - \mu_2) g_y(y) dy = 0$$

If (X,Y) have a bivariate **normal** distribution, then  $cov(X,Y) = 0 \Rightarrow X,Y$  independent

In general, cov(X,Y) measures the **association** between X and Y, i.e. the extent to which X and Y vary together

Large X occurs with large Y and small X occurs with small Y  $\Leftrightarrow$  **positive** association Large X occurs with small Y and small X occurs with large Y  $\Leftrightarrow$  **negative** association

Sample covariance = 
$$\frac{1}{n-1}\sum (x_i - \bar{x})(y_i - \bar{y})$$
 estimates  $cov(X,Y)$ 

If 
$$(x_i - \bar{x}) > 0$$
 and  $(y_i - \bar{y}) > 0$  then  $(x_i - \bar{x}) (y_i - \bar{y}) > 0$ 

If 
$$(x_i - \bar{x}) < 0$$
 and  $(y_i - \bar{y}) < 0$  then  $(x_i - \bar{x}) (y_i - \bar{y}) > 0$ 

Positive association between X and Y  $\Leftrightarrow$  sample covariance > 0

If 
$$(x_i - \bar{x}) > 0$$
 and  $(y_i - \bar{y}) < 0$  then  $(x_i - \bar{x}) (y_i - \bar{y}) < 0$ 

If 
$$(x_i - \bar{x}) < 0$$
 and  $(y_i - \bar{y}) > 0$  then  $(x_i - \bar{x}) (y_i - \bar{y}) < 0$ 

Negative association between X and Y  $\Leftrightarrow$  sample covariance < 0

Sign of sample covariance indicates the direction of association: positive or negative

### Properties of sample correlation coefficient $r_{XY}$

$$r_{XY} \ = \frac{SXY}{\sqrt{(SXX)(SYY)}} \ = \frac{SXY \, / \, (n-1)}{\sqrt{(SXX \, / \, (n-1))(SYY \, / \, (n-1))}}$$

Where 
$$\begin{aligned} SXY &= \sum (x_i - \overline{x})(y_i - \overline{y}) = \sum x_i y_i - n \overline{x} \, \overline{y} \\ SXX &= \sum (x_i - \overline{x})^2 = \sum x_i^2 - n(\overline{x})^2 \\ SYY &= \sum (y_i - \overline{y})^2 = \sum y_i^2 - n(\overline{y})^2 \end{aligned}$$

Correlation coefficient  $r_{XY}$  is the sample covariance, scaled to lie in [-1, 1]

$$-1 <= r_{XY} <= 1$$

 $r_{XY} > 0 \Leftrightarrow$  positive association;  $r_{XY} < 0 \Leftrightarrow$  negative association

 $r_{XY} = 1 \Leftrightarrow$  all points lie on line with positive slope

 $r_{XY} = -1 \Leftrightarrow$  all points lie on line with negative slope

The closer  $r_{XY}$  is to +1, the closer the points are to a line with positive slope

The closer  $r_{XY}$  is to -1, the closer the points are to a line with negative slope

In simple regression, r (or its square  $r^2$ ) is used to measure how well the linear model fits the data

In multiple regression, the multiple correlation coefficient (R<sup>2</sup>) is used to measure how well the linear model fits the data

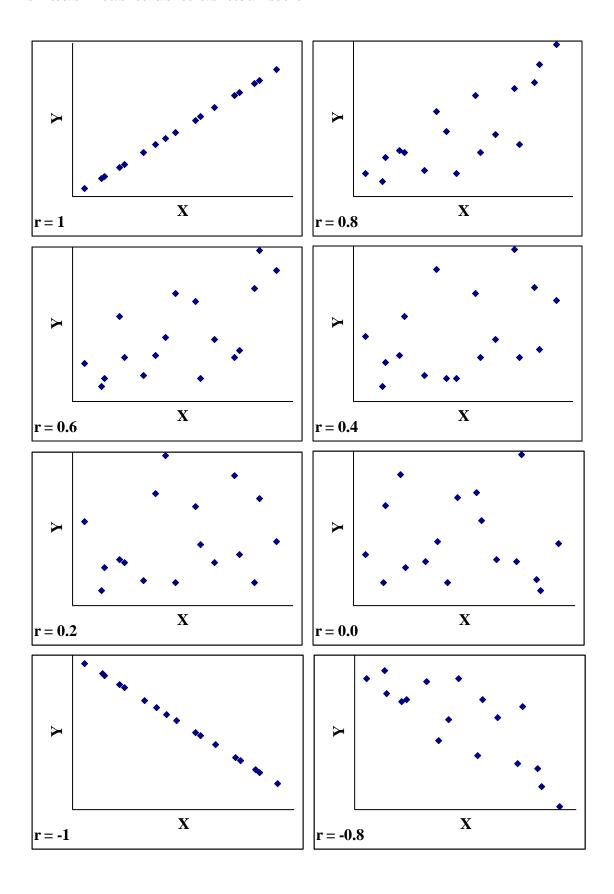
For the Forbes data,

$$\overline{x} = 202.95 \qquad \overline{y} = 139.61$$

$$SXX = 530.78$$
  $SXY = 475.30$   $SYY = 427.76$ 

(You should verify these results using a calculator/spreadsheet/R as an exercise)

$$r_{XY} = \frac{475.30}{\sqrt{(530.78)(427.76)}} = 0.9975$$

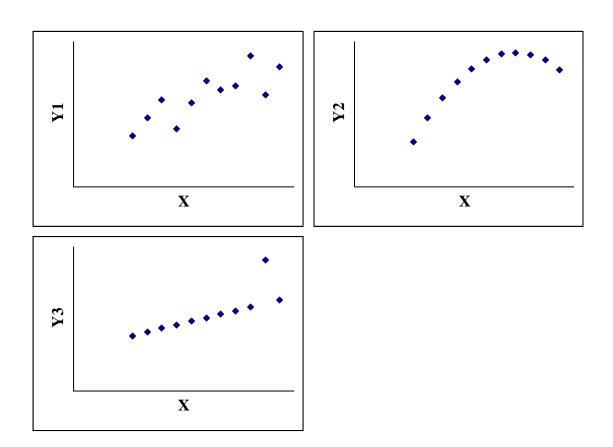


Linearity cannot be deduced from the correlation coefficient. The correlation coefficient should never be interpreted in isolation – but in conjunction with the scatter-plot:

X	Y1	Y2	Y3
10	8.04	9.14	7.46
8	6.95	8.14	6.77
13	7.58	8.74	12.74
9	8.81	8.77	7.11
11	8.33	9.26	7.81
14	9.96	8.10	8.84
6	7.24	6.13	6.08
4	4.26	3.10	5.39
12	10.84	9.13	8.15
7	4.82	7.26	6.42
5	5.68	4.74	5.73
r =	0.82	0.82	0.82

All give the same r – this may lead us to believe that each of these Y's has the same relationship with X.

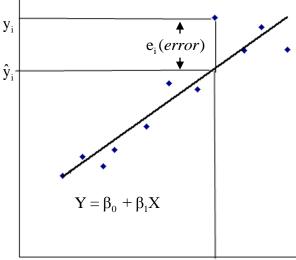
But consider the scatter-plots:



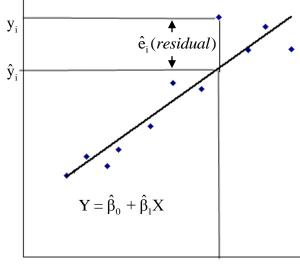
## **Least Squares Criterion:**

In a scatter plot there may be many potential lines that could be fitted to the data. The method for choosing the best line is the Least Squares Criterion.

## True regression line:



## **Fitted regression line:**



Chose  $\hat{\beta}_0$  and  $\hat{\beta}_1$  to minimize the sum of the squared residuals (  $\sum_{i=1}^n \hat{e}_i^2$  ).

RSS (Residual Sum of Squares) is the (minimized) value of  $\sum_{i=1}^{n} \hat{e}_{i}^{2}$ .

 $\mathbf{X}_{i}$ 

Through partial differentiation, the following estimators can be derived:

$$\hat{\beta}_1 = \frac{SXY}{SXX} \quad \hat{\beta}_0 = \overline{y} - \hat{\beta}_1 \overline{x}$$

## Derivation of regression coefficient estimators (for ST2053 and ST6018 only)

$$RSS = \sum_{i=1}^{n} \hat{\mathbf{e}}_{i}^{2} = \sum_{i=1}^{n} (y_{i} - (\hat{\boldsymbol{\beta}}_{0} + \hat{\boldsymbol{\beta}}_{1} x_{i}))^{2}$$
 Note: the index on the summation sign is dropped for simplicity.

To minimize RSS, we need to differentiate with respect to 2 unknowns – we need the partial derivatives.

We set these partial derivatives equal to zero and solve the (simultaneous) equations.

(Remember that  $y_i$  and  $x_i$  are known (the data) and that  $\hat{\beta}_0$  and  $\hat{\beta}_1$  are the unknowns.)

$$\frac{\delta RSS}{\delta \hat{\beta}_0} = 2\sum (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)(-1) = 0$$

$$\frac{\delta RSS}{\delta \hat{\beta}_1} = 2\sum (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)(-x_i) = 0$$

$$\sum (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i) = 0$$

$$\sum (x_i y_i - \hat{\beta}_0 x_i - \hat{\beta}_1 x_i^2) = 0$$

$$\sum y_i = \sum \hat{\beta}_0 + \sum \hat{\beta}_1 x_i$$

$$\sum x_i y_i = \sum \hat{\beta}_0 x_i + \sum \hat{\beta}_1 x_i^2$$

$$\sum x_i y_i = \hat{\beta}_0 \sum x_i + \hat{\beta}_1 \sum x_i^2$$

This is called the 1<sup>st</sup> normal equation.

This is called the  $2^{nd}$  normal equation.

To solve these simultaneous equations:

Multiply each term in the 1<sup>st</sup> normal equation by  $-\sum x_i$  and every term in the 2<sup>nd</sup> normal equation by n and add:

$$-\sum_{i} x_{i} \sum_{j} y_{i} = -n\hat{\beta}_{0} \sum_{j} x_{i} - \hat{\beta}_{1} (\sum_{j} x_{i})^{2}$$

$$\underline{n} \sum_{i} x_{i} y_{i} = n\hat{\beta}_{0} \sum_{j} x_{i} + n\hat{\beta}_{1} \sum_{j} x_{i}^{2}$$

$$\underline{n} \sum_{i} x_{i} y_{i} - \sum_{i} x_{i} \sum_{j} y_{i} = n\hat{\beta}_{1} \sum_{i} x_{i}^{2} - \hat{\beta}_{1} (\sum_{j} x_{i})^{2} \quad \text{(This eliminated } \hat{\beta}_{0})$$

$$\underline{n} \sum_{i} x_{i} y_{i} - \sum_{i} x_{i} \sum_{j} y_{i} = \hat{\beta}_{1} (n \sum_{j} x_{i}^{2} - (\sum_{j} x_{i})^{2})$$

$$\underline{n} \sum_{i} x_{i} y_{i} - \sum_{j} x_{i} \sum_{j} y_{i} = n \sum_{j} x_{i} \sum_{j} y_{i} \quad \text{Remember } \overline{x} = \frac{\sum_{j} x_{i}}{n}, \text{ similarly for } \overline{y}$$

$$\hat{\beta}_{1} = \frac{n \sum_{j} x_{i} y_{i} - n \overline{x} n \overline{y}}{n \sum_{j} x_{i}^{2} - (n \overline{x})^{2}} \quad \text{Can cancel } n:$$

$$\hat{\beta}_{1} = \frac{\sum_{j} x_{i} y_{i} - n \overline{x} \overline{y}}{\sum_{j} x_{i}^{2} - n(\overline{x})^{2}} = \frac{\mathbf{SXY}}{\mathbf{SXX}}$$

Consider the 1st normal equation:

$$\sum y_i = n\hat{\beta}_0 + \hat{\beta}_1 \sum x_i$$

$$n\hat{\beta}_0 = \sum y_i - \hat{\beta}_1 \sum x_i$$
 Divide each term by  $n$ :
$$\hat{\beta}_0 = \overline{y} - \hat{\beta}_1 \overline{x}$$

Note: The proof that the solution to the normal equations provides a minimum rather than a maximum is omitted.

For the Forbes data,

$$\hat{\beta}_1 = \frac{475.30}{530.78} = 0.8955 \ \hat{\beta}_0 = 139.61 - (0.8955)(202.95) = -42.131$$
 (Can you verify these results?)

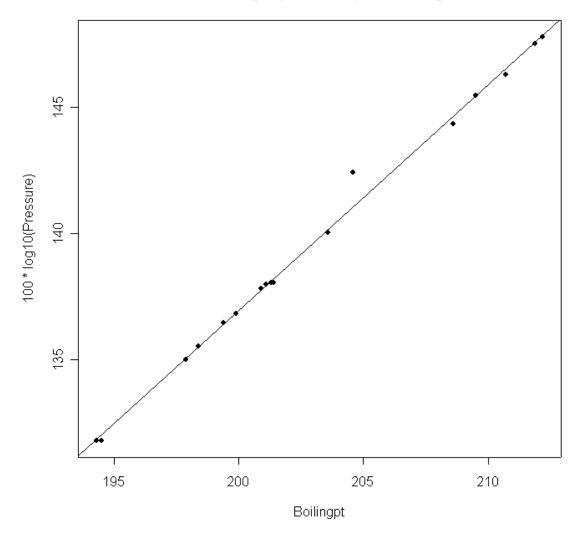
Fitted regression model: 100\*log(Pressure) = -42.131 + 0.8955 Boiling Pt

Case	Boiling Pt (°F)	100*Log(Pressure)	Fitted Value	Residual
	<u> </u>	<u> </u>		
1	194.5	131.79	132.04	-0.2481
2	194.3	131.79	131.86	-0.0690
3	197.9	135.02	135.09	-0.0538
4	198.4	135.55	135.54	0.0187
5	199.4	136.46	136.43	0.0330
6	199.9	136.83	136.88	-0.0412
7	200.9	137.82	137.77	0.0561
8	201.1	138.00	137.95	0.0584
9	201.4	138.06	138.22	-0.1560
10	201.3	138.04	138.13	-0.0845
11	203.6	140.04	140.19	-0.1471
12	204.6	142.44	141.09	1.3599
13	209.5	145.47	145.48	0.0014
14	208.6	144.34	144.67	-0.3198
15	210.7	146.30	146.55	-0.2429
16	211.9	147.54	147.63	-0.0792
17	212.2	147.80	147.89	-0.0871

Estimate of common variance (
$$\sigma^2$$
):  $\hat{\sigma}^2 = \frac{RSS}{n-2} = \frac{2.1579}{17-2} = 0.1439$ 

Fitted regression line for Forbes data:

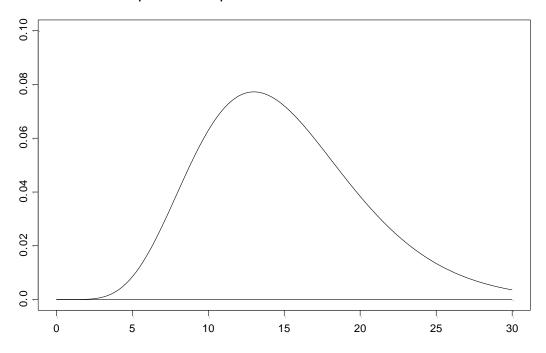
# Plot of 100\*log10(Pressure) vs. Boiling Point



## The $\chi^2$ (chi-squared) distribution

There is a family of  $\chi^2$  variables with different degrees of freedom (df), denoted by v.  $\chi^2(v)$  denotes a chi–squared variable with v df, for v=1, 2, 3,...,

pdf of chi-squared distribution with 15 df



It may be shown that  $E(\chi^2(v)) = v$ , so  $E(\chi^2(n-2)) = n-2$  and  $E(\chi^2(15)) = 15$ 

It may be shown that  $\frac{RSS}{\sigma^2} \sim \chi^2(n-2)$ , so  $E(\frac{RSS}{\sigma^2}) = n-2$  and so  $E(\frac{RSS}{n-2}) = \sigma^2$ Thus  $\frac{RSS}{n-2}$  is an **unbiased** estimate of  $\sigma^2$ 

Here n = number of pairs of observations = 17 and RSS = 2.1579.

So and unbiased estimate of  $\sigma^2$  is  $\frac{2.1579}{17-2} = 0.1439$ 

and  $\sqrt{0.1439} = 0.3793$  is an estimate of  $\sigma$  and is called the **standard error of regression** (or the **residual standard error** in R).

## Example of standard error: the sampling distribution of the mean

If  $X_1, X_2,... X_n$  are IID with  $E(X_i) = \mu$  and var  $(X_i) = \sigma^2$ ,

then 
$$\overline{X}=\frac{1}{n}\sum_{i=1}^n X_i$$
 has mean  $E(\overline{X})=\mu$  and variance  $var(\overline{X})=\frac{\sigma^2}{n}$ 

The sample variance  $s^2 = \frac{1}{n-1} \sum_{i=1}^{n} (X_i - \overline{X})^2$  is an unbiased estimate of  $\sigma^2$ 

Hence  $\frac{s^2}{n}$  is an unbiased estimate of  $var(\overline{X}) = \frac{\sigma^2}{n}$ 

and so 
$$\frac{s}{\sqrt{n}} = \sqrt{\frac{s^2}{n}}$$
 is an estimate of  $sd(\overline{X}) = \frac{\sigma}{\sqrt{n}}$ 

 $\frac{s}{\sqrt{n}}$  is called the **standard error of the mean** and denoted by  $se(\overline{X})$ 

#### In general, the square root of an estimated variance is called a standard error

#### **Analysis of Variance**

$$SYY = \sum_{i=1}^{n} (y_i - \bar{y})^2 = \text{total sum of squares for the } y_i's$$

SYY measures the total variability of the yi's about their mean

RSS = residual sum of squares = sum of squared residuals

RSS measures that part of the total variability of the y<sub>i</sub>'s **not explained** by the regression line

## **Regression Sum of Squares** = SSreg = SYY - RSS

SSreg measures that part of the total variability of the y<sub>i</sub>'s **explained** by the regression line

SSreg can be calculated directly from SSreg = 
$$\frac{(SXY)^2}{SXX}$$

The fundamental identity of the analysis of variance is

$$SYY = SSreg + RSS$$

Total sum of squares = regression sum of squares + residual sum of squares

For a **perfect fit**, RSS = 0 and SYY = SSreg

## The Coefficient of Determination, R<sup>2</sup>

The proportion of variability that is explained can be expressed as a percentage of the total variability in the Y's – called the Coefficient of Determination,  $R^2$ .

$$R^2 = \frac{\text{SSreg}}{\text{SYY}} = \frac{\text{SYY} - \text{RSS}}{\text{SYY}} = \frac{427.76 - 2.1579}{427.76} = 99.50\%$$

Here, 99.50% of the variability in the observed 100\*log(pressure) values can be explained by the boiling point.

What would a low value of R<sup>2</sup> mean?

In the case of simple linear regression,  $R^2 = r^2$ .  $R^2 = (0.9975)^2 = 99.50\%$ 

### The F-test for regression

Our regression model is

$$y_i \; = \; \beta_0 \, + \beta_1 \, x_i + e_i$$

We test the **null hypothesis**  $H_0$ :  $\beta_1 = 0$ against the **alternative hypothesis**  $H_1: \beta_1 \neq 0$ 

 $H_0$  says that the **true** regression line is **horizontal** ( $y_i = \beta_0 + e_i$ )

In this case, the least squares estimate of  $\beta_0$  is  $\overline{y}$  and each fitted value is  $\hat{y}_i = \overline{y}$  and so

$$SYY = \sum (y_i - \overline{y})^2 = \sum (y_i - \hat{y}_i)^2 = RSS$$

If H<sub>0</sub> is true, then X is **no use** in predicting Y and X **should not** be included in the regression model.

H<sub>1</sub> says that the true regression line is **not horizontal** and so X is **of use** in predicting Y and **should** be included in the regression model.

Intuitively, the more the fitted line differs from a horizontal line and the more of SYY that is explained by the regression, the more we should be inclined to reject H<sub>0</sub> and accept H<sub>1</sub>, i.e. to conclude that X is worth including in the regression model.

Here the fitted line is far from horizontal and SSreg = 425.61 accounts for most of SYY = 427.76, which strongly suggests that we should reject H<sub>0</sub> and accept H<sub>1</sub>.

If H<sub>0</sub> is true, it may be shown that  $E(SSreg/1) = E(RSS/(n-2)) = \sigma^2$ 

Thus, if  $H_0$  is true, the Regression Mean Square is also an unbiased estimate of  $\sigma^2$  and so we would expect the Regression Mean Square and the Residual Mean Square to be about the same size

If H<sub>1</sub> is true, it may be shown that  $E(SSreg/1) > \sigma^2$ , so we would expect the Regression Mean Square to be bigger than the Residual Mean Square

Here SSreg/1 = 425.60 while RSS/(n-2) = 0.1439.

Thus the Regression Mean Square is much bigger than the Residual Mean Square and this provides strong evidence that H<sub>1</sub> is true and H<sub>0</sub> is false

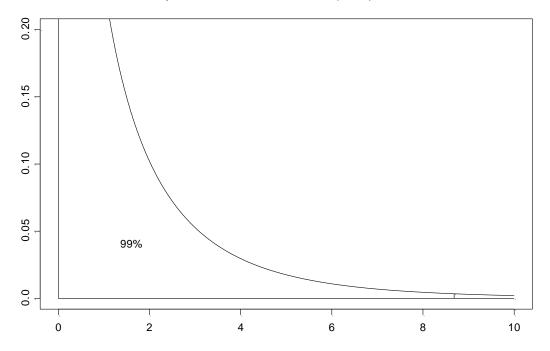
If H<sub>0</sub> is true, it may be shown that 
$$F = \frac{SSreg/1}{RSS/(n-2)} \sim F(1,n-2)$$

If the observed value of F is **too big**, we reject  $H_0$  and accept  $H_1$ .

## The F-distribution

There is a family of F variables, each with a pair of degrees of freedom  $v_1$  and  $v_2$ .

pdf of F-distribution with (1,15) df



Critical values of F for specified significance levels (e.g.  $\alpha = 0.01$ ) are found in F- tables

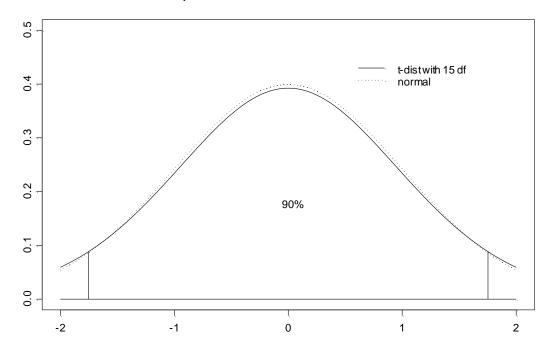
$v_1 = 1$	
$v_2 = 14$	8.86
$v_2 = 15$	8.68
$v_2 = 16$	8.53

Here F(0.01;1,15) = 8.68, while the observed value of F is 2958. Thus is the observed value of F is significant at the 1% significance level. The observed p-value << 0.01.

#### The t-distribution

There is a family of t-variables with different degrees of freedom (df). Let t(v) denote a t-variable with v degrees of freedom. The pdf for t(v) is similar in shape to that of the N(0,1) distribution, but flatter. As  $v \to \infty$ , the  $t(v) \to N(0,1)$ .

## pdf of t-distribution with 15 df



Critical values for t-distributions are found in t-tables.

$$\alpha = 0.05$$
  $v = 15$   $t = 1.753$ 

Thus 5% of the area under the pdf curve of t(15) lies in the interval  $(1.753, \infty)$  and 5% of the area lies in the interval  $(\infty, -1.753)$  and 90% of the area lies in the interval (-1.753, 1.753). Thus each tail of the distribution accounts for 5% of the area under the pdf.

Let  $t(\alpha, n-1) = \text{critical}$  value of t-distribution with df = n-1 for a two-sided test with significance level  $\alpha$ , i.e. an area of  $\alpha/2$  in each tail.

$$t(0.10, 15) = 1.753$$
  $t(0.05, 15) = 2.131$   $t(0.01, 15) = 2.947$ 

## t-tests and confidence intervals:

#### **Population mean:**

If 
$$X_1, X_2, \ldots X_n$$
 are NID( $\mu, \sigma^2$ ), then  $\frac{\overline{X} - \mu}{s / \sqrt{n}} = \frac{\overline{X} - E(\overline{X})}{se(\overline{X})} \sim t_{n-1}$ 

The general form in which the t-distribution occurs is:  $\frac{\text{variable} - \text{E(variable)}}{\text{se(variable)}} \sim t$ 

To test the hypothesis H<sub>0</sub>:  $\mu = \mu_0$  against H<sub>1</sub>:  $\mu \neq \mu_0$ , use the test statistic  $t = \frac{\overline{X} - \mu_0}{s / \sqrt{n}}$ 

If the  $|t|>t(\alpha,\,n\text{-}1)$ , reject  $H_0$ :  $\mu=\mu_0$  and accept  $H_1$ :  $\mu\neq\mu_0$ . This test has significance level  $\alpha$ .

The general form for a test statistic based on the t-distribution is

$$t = \frac{variable - E(variable)}{se(variable)}$$

The  $(1 - \alpha)100\%$  confidence interval for  $\mu$  is :  $\overline{X} \pm t(\alpha, n-1) \frac{s}{\sqrt{n}}$ 

The general form for a  $(1 - \alpha)100\%$  confidence interval based on the t-distribution is

variable  $\pm$  t( $\alpha$ , df) se(variable)

#### **Prediction and fitted values**

To predict the actual value of Y at a given value of X, we use the fitted value. Let se<sub>pred</sub>= standard error of this prediction.

$$se_{pred} = \sigma \sqrt{1 + \frac{1}{n} + \frac{(X_p - \overline{X})^2}{SXX}}$$
. We replace  $\sigma$  by its estimate sqrt(RSS/(n-2)) to get an estimated standard error.

To estimate the average value of Y at a given value of X, we use the fitted value. Let  $se_{fit} = standard$  error of the fitted value, when used to estimate the average value of Y for given X.

$$se_{fit} = \sigma \sqrt{\frac{1}{n} + \frac{(X_p - \bar{X})^2}{SXX}}$$
. We again replace  $\sigma$  by its estimate  $sqrt(RSS/(n-2))$  to get an estimated standard error.

For the Forbes data, estimate the average Y value (100\*log(Pressure)) for a Boiling point of 200.

Fitted regression model: 100\*log(Pressure) = -42.131 + 0.8955 Boiling Pt Fitted value: 100\*log(Pressure) = -42.131 + 0.8955 (200) = 136.969

A  $(1 - \alpha)100\%$  confidence interval for average value of Y at a given value of X is given by: fitted value  $\pm$  t( $\alpha$ , n-2) se(fitted value)

$$se_{fit} = \hat{\sigma}\sqrt{\frac{1}{n} + \frac{(X_p - \overline{X})^2}{SXX}} = 0.3793\sqrt{\frac{1}{17} + \frac{(200 - 202.95)^2}{530.78}} = 0.1040$$

A 99% confidence interval is  $136.969 \pm 2.947(0.1040) = (136.663, 137.275)$ 

#### Residuals

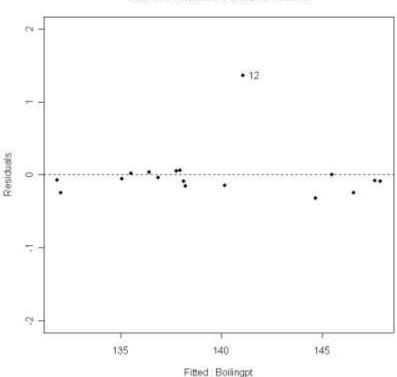
The residuals can be used to check the assumptions about the error terms and to check the appropriateness of the model.

There are many ways in which the residual are used and these will be the focus of later chapters.

For now, we concentrate on a plot of the residuals versus the fitted values.

Curvature in this plot would suggest that the relationship is not linear and a transformation of one or both variables would be beneficial.

The common variance assumption would be violated if the residuals appeared to increase (or decrease) in magnitude with the predicted values.



#### Plot of residuals vs. fitted values

There does not appear to be any curvature.

The common variance appears constant.

The residual for case 12 is very large relative to the others. It might suggest that the assumptions about the errors are not correct.

- Recording/measurement error in case 12? Investigate?
- Impact of including/excluding case 12?

### **Previous Exam Question 1**

Data were obtained on the lean body mass (the weight without fat in kg) and resting metabolic rate for twelve women who were the subjects in a study of obesity. The scatter plot showed evidence of a linear relationship within the range of the data.

A model of the following form was fitted to these data:

$$Y_i = \beta_0 + \beta_1 X_i + e_i, e_i \sim \text{NID}(0, \sigma^2),$$

where Y = Rate = resting metabolic rate and X = Bodymass = lean body mass.

Excerpts from the R output for this model are shown on the next page.

- (a) Identify the estimate of  $\beta_1$  and interpret it.
- (b) Interpret the value of *R*-Squared.
- (c) Test the hypothesis  $H_0$ :  $\beta_1 = 0$  against  $H_1$ :  $\beta_1 \neq 0$ . Quote the value of the test statistic and the associated *p*-value. Outline the practical implications of your conclusion.

(d) Find a 95% confidence interval for  $\beta_1$ . Comment on the implications of this interval for part (c).

(e) Find a 95% confidence interval for the mean resting metabolic rate of women with a lean body mass of (i) 50kg and (ii) 75kg. Comment on the <u>appropriateness</u> of the intervals in each case.

## R output for Question 1

```
> summary(bodymass.lm)
Call:
lm(formula = Rate ~ Bodymass)
Coefficients:
           Estimate Std. Error t value Pr(>|t|)
(Intercept) 201.162 181.701 1.107 0.294169
          24.026
                       4.174 5.756 0.000184 ***
Bodymass
___
Signif. codes: 0 `***' 0.001 `**' 0.01 `*' 0.05 `.' 0.1 `
1 1
Residual standard error: 95.08 on 10 degrees of freedom
Multiple R-Squared: 0.7682, Adjusted R-squared: 0.745
F-statistic: 33.13 on 1 and 10 DF, p-value: 0.0001836
> qt(0.975,10)
[1] 2.228139
> predict(bodymass.lm,
data.frame(Bodymass=c(50,75)), se.fit=T,
interval="confidence", level = 0.95)
$fit
      fit
               lwr
1 1402.465 1313.370 1491.560
2 2003.117 1699.602 2306.631
$se.fit
       1
 39.98617 136.21886
> summary(bodymass.df)
   Bodymass
                    Rate
Min.
       :33.10 Min.
                      : 913
1st Qu.:39.25 1st Qu.:1106
Median :42.00 Median :1230
Mean :43.03 Mean :1235
 3rd Qu.:49.02 3rd Qu.:1402
Max. :54.60
                Max. :1502
```

# Practical (Assignment) 1

## Instructions for this practical

- Open the template "Surname Forename Chpt x" from Canvas (in "Practicals").
- Complete the grid on the first page.
- Save this file (as a Word document) using your own surname, forename and the appropriate chapter number.
- Practice Question:
- Type the commands one by one into R.
- Compare the results in the R text output and graphics with the corresponding results and figures in your notes.
- Use appropriate R output to answer the questions, adapting the R code if necessary.
- Exam Question:
- Adapt the relevant R code you used for the practice question to answer the questions.
- Copy and paste the relevant R text output and graphics into your Word document to support your answers. Change the text font to "Courier New" to align columns.
- Restrict your Word document to a **maximum of 2 pages** (re-sizing graphics and deleting irrelevant R output will help).
- Submit this Word document **via Canvas** by **5.00pm** \_\_\_\_\_\_(STRICT deadline)
- Note that submitting the practical is a declaration that the practical is your own work. Plagiarism/copying will not be tolerated.

#### **Practice Question (not to be submitted)**

Data on the Boiling Point of water (°F) and Atmospheric Pressure (in. Hg) were recorded at 17 locations in the **forbes.txt** dataset. Fit a model of the following form to this data:

$$Y_i = \beta_0 + \beta_1 X_i + \varepsilon_i, \varepsilon_i \sim IN(0,\sigma^2),$$

where  $Y = 100 \log(Pressure)$  and X = Boiling Point.

- (a) Identify the estimate of  $\beta_1$  and interpret it.
- (b) Interpret the value of R-Squared.
- (c) Test the hypothesis  $H_0$ :  $\beta_1 = 0$  against  $H_1$ :  $\beta_1 \neq 0$ . Outline the practical implications of your conclusion.
- (d) Find 99% confidence intervals for  $\beta_0$  and  $\beta_1$ .
- (e) Find a 99% confidence interval for the mean value of Y for X = 200.
- (f) Find a 99% prediction interval for the value of Y for X = 200.

#### **Exam Question (Winter 2020-21, Question 1) (to be submitted)**

Data were collected on a random sample of adults who were undergoing a physical examination. The data are stored in **BMI.txt** (on Canvas & P: drive).

Fit a model of the following form to these data:

- (a) Provide an appropriate scatter-plot for these data. Comment on this plot. (15 marks)
- (b) Calculate a 95% confidence interval for the slope. Interpret this confidence interval. (10 marks)
- (c) Test the hypothesis  $H_0$ :  $\beta_1 = 0.3$  against  $H_1$ :  $\beta_1 \neq 0.3$ . Quote the value of the test statistic and the associated p-value. (15 marks)
- (d) Predict the BMI of an adult with a waist circumference 88cm. Interpret the associated 95% confidence interval. (10 marks)

```
# R code and output for Chapter 1
> # read in Forbes data
> forbes.df <-
read.table("P:\\ST2053\\forbes.txt",header=T
)
> forbes.df
   Boilingpt Pressure
1
       194.5
                 20.79
2
       194.3
                 20.79
3
       197.9
                 22.40
4
       198.4
                 22.67
5
       199.4
                 23.15
6
       199.9
                 23.35
7
       200.9
                 23.89
8
       201.1
                 23.99
9
                 24.02
       201.4
10
       201.3
                 24.01
11
       203.6
                 25.14
12
       204.6
                 26.57
13
       209.5
                 28.49
14
       208.6
                 27.76
15
       210.7
                 29.04
16
       211.9
                 29.88
17
       212.2
                 30.06
```

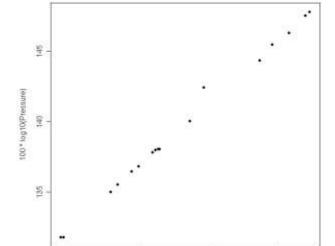
Note: you will need to change P:\\ST2053\\ to the appropriate path on your own computer at which you saved the forbes.txt file from Canvas.

This applies to all such paths throughout these notes.

### > attach(forbes.df)

> # Scatter plot

> plot(Boilingpt, 100\*log10(Pressure), main="Plot of 100\*log10(Pressure) vs. Boiling Point", pch=16)



205

Boilingpt

210

200

#### Plot of 100\*log10(Pressure) vs. Boiling Point

- > # Fit regression line
- > forbes.lm <- lm(100\*log10(Pressure)~ Boilingpt)</pre>

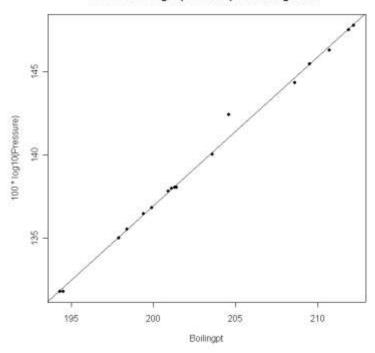
#### > coef(forbes.lm)

(Intercept) Boilingpt -42.1641838 0.8956178

- > # Scatter plot with fitted line
- > plot(Boilingpt, 100\*log10(Pressure), main="Plot of 100\*log10(Pressure) vs. Boiling Point", pch=16)

#### > abline(forbes.lm)

#### Plot of 1001og10(Pressure) vs. Boiling Point



```
> # Residual standard error
> # Multiple R-squared
> # Standard errors of regression coefficients
> summary(forbes.lm)
Call:
lm(formula = 100 * log10(Pressure) ~ Boilingpt)
Residuals:
    Min
           1Q Median 3Q Max
-0.31974 -0.14707 -0.06890 0.01877 1.35994
Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) -42.16418 3.34136 -12.62 2.17e-09 ***
Boilingpt 0.89562
                       0.01646 54.42 < 2e-16 ***
Signif. codes: 0 `***' 0.001 `**' 0.01 `*' 0.05 `.' 0.1 `
1 1
Residual standard error: 0.3792 on 15 degrees of freedom
Multiple R-Squared: 0.995, Adjusted R-squared: 0.9946
F-statistic: 2962 on 1 and 15 DF, p-value: < 2.2e-16
> # critical value of t-distribution
> qt(0.95,15)
[1] 1.753050
> # 90% confidence limits for beta-0
> -42.16418 + (qt(0.95,15)*3.34136)
[1] -36.30661
> -42.16418 - (qt(0.95,15)*3.34136)
[1] -48.02175
> # 90% confidence limits for beta-1
> 0.89562 + (qt(0.95,15)*0.01646)
[1] 0.9244752
> 0.89562 - (qt(0.95,15)*0.01646)
[1] 0.8667648
```

```
> # Anova table, F-test
> anova(forbes.lm)
Analysis of Variance Table
Response: 100 * log10(Pressure)
         Df Sum Sq Mean Sq F value Pr(>F)
Boilingpt 1 425.76 425.76 2961.5 < 2.2e-16 ***
Residuals 15 2.16 0.14
Signif. codes: 0 `***' 0.001 `**' 0.01 `*' 0.05 `.' 0.1 `
1 1
> # 99% confidence interval for the mean of y
> predict(forbes.lm, data.frame(Boilingpt=200),se.fit=T,
interval="confidence",level=0.99)
$fit
          fit lwr upr
[1,] 136.9594 136.6529 137.2659
$se.fit
[1] 0.1040112
$df
[1] 15
$residual.scale
[1] 0.3791592
> # critical value of t-distribution
> qt(0.995,15)
[1] 2.946713
> # alternative derivation of
> # 99% confidence interval for the mean of y
> 136.9594 + (qt(0.995,15)*0.104)
[1] 137.2659
> 136.9594 - (qt(0.995,15)*0.104)
[1] 136.6529
```

> # 99% prediction interval for individual value of y
> predict(forbes.lm, data.frame(Boilingpt=200),se.fit=T,
interval="prediction",level=0.99)
\$fit

fit lwr upr [1,] 136.9594 135.8008 138.1179

#### \$se.fit

[1] 0.1040112

#### \$df

[1] 15

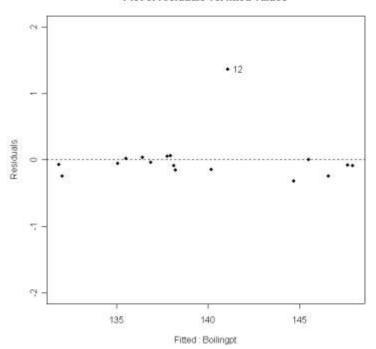
#### \$residual.scale

[1] 0.3791592

> # Plot of residuals vs. fitted values
> plot(fitted(forbes.lm), resid(forbes.lm), main="Plot of
residuals vs. fitted values", xlab="Fitted :
Boilingpt",ylab="Residuals", ylim=c(-2,2),pch=16)

> abline(h=0,lty=2)

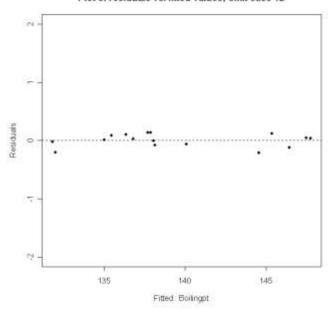
#### Plot of residuals vs. fitted values



```
> # Omitting a case
> # identify outlier
> outlier <-
identify(fitted(forbes.lm),resid(forbes.lm),n=1)
> outlier
[1] 12
> subset.forbes.lm <- lm(100*log10(Pressure)~ Boilingpt,
subset = -outlier)
> summary(subset.forbes.lm )
```

```
Call:
lm(formula = 100 * log10(Pressure) ~ Boilingpt, subset = -
outlier)
Residuals:
     Min
              1Q Median
                                3Q
                                        Max
-0.20882 -0.06338 0.01974 0.08842 0.13558
Coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept) -41.334683 1.003312 -41.2 5.16e-16 ***
Boilingpt 0.891110 0.004944 180.2 < 2e-16 ***
Signif. codes: 0 `*** 0.001 `** 0.01 `* 0.05 `. 0.1 `
Residual standard error: 0.1136 on 14 degrees of freedom
Multiple R-Squared: 0.9996, Adjusted R-squared: 0.9995
F-statistic: 3.249e+04 on 1 and 14 DF, p-value: < 2.2e-16
> # Plot of residuals vs.fitted values
> plot(fitted(subset.forbes.lm), resid(subset.forbes.lm),
main="Plot of residuals vs. fitted values; omit case 12",
xlab="Fitted : Boilingpt",ylab="Residuals",ylim=c(-2,2),
pch=16)
> abline(h=0,lty=2)
```





> # quit R > q("yes")