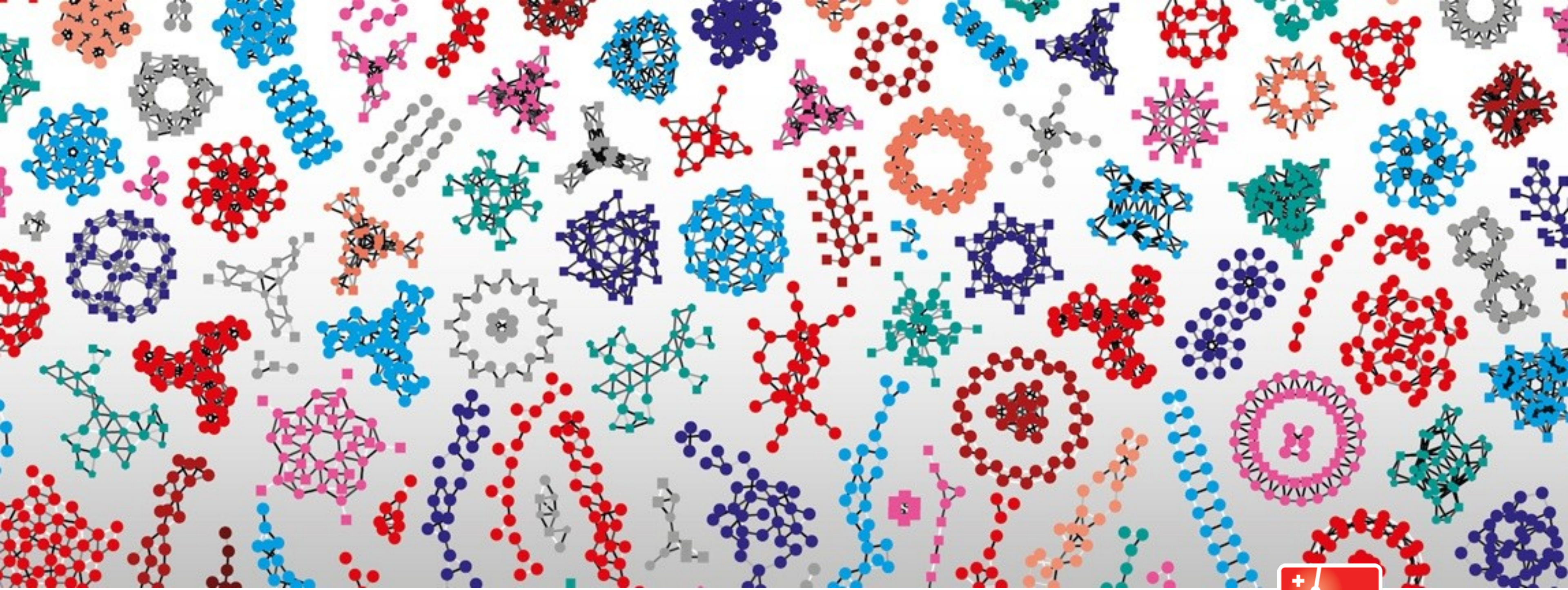


Swiss Institute of Bioinformatics

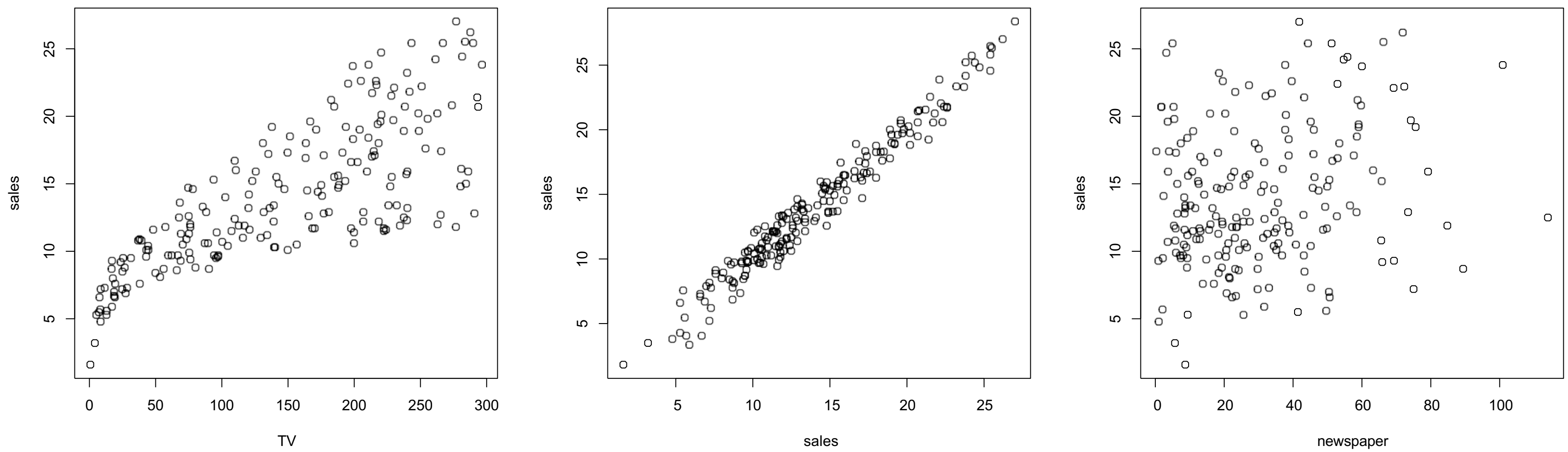
Introduction to statistics

Lausanne, 08-11 February 2021

Isabelle Dupanloup, Rachel Marcone

Day 3:
Correlation and Regression

Scatterplot

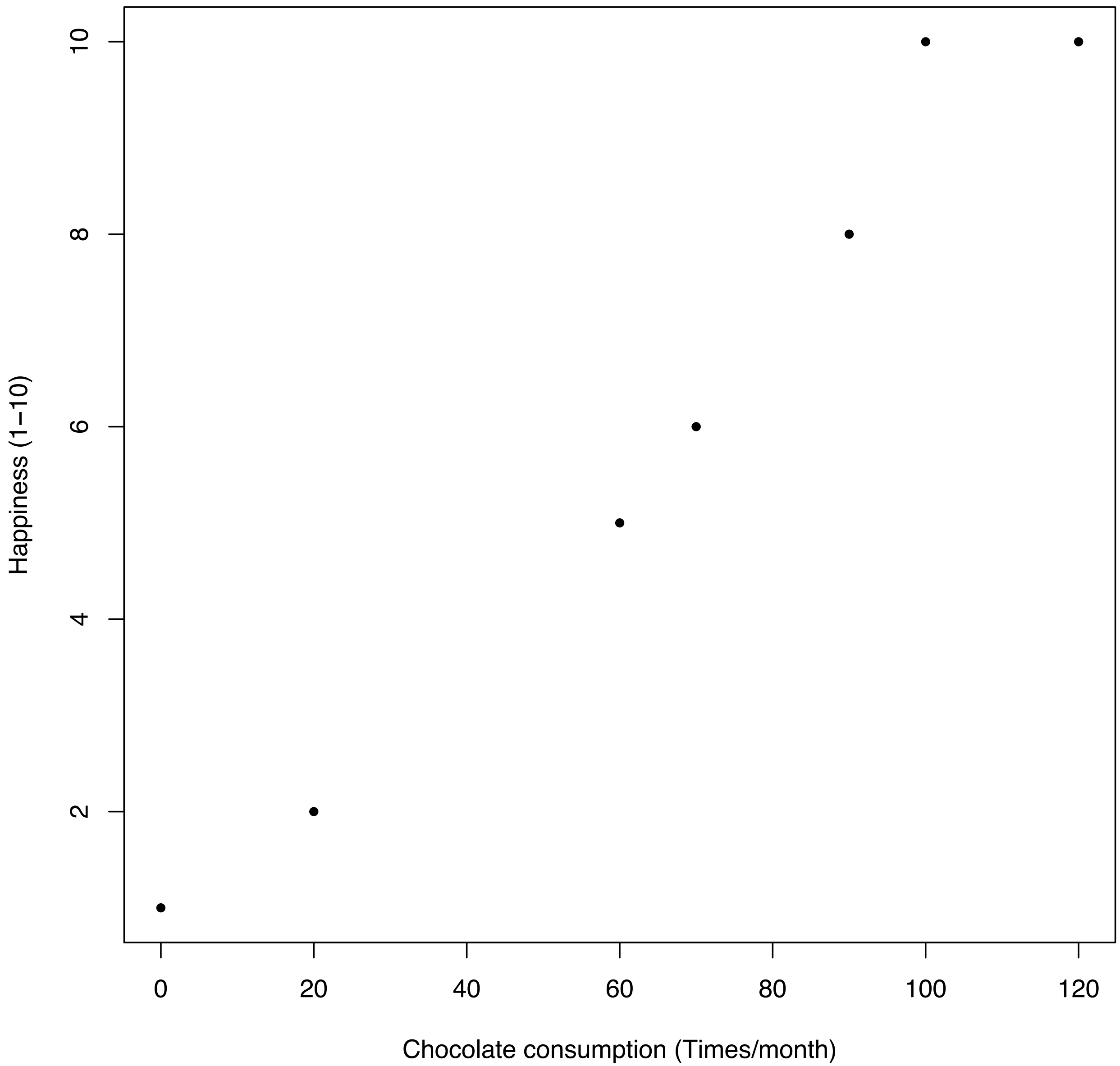


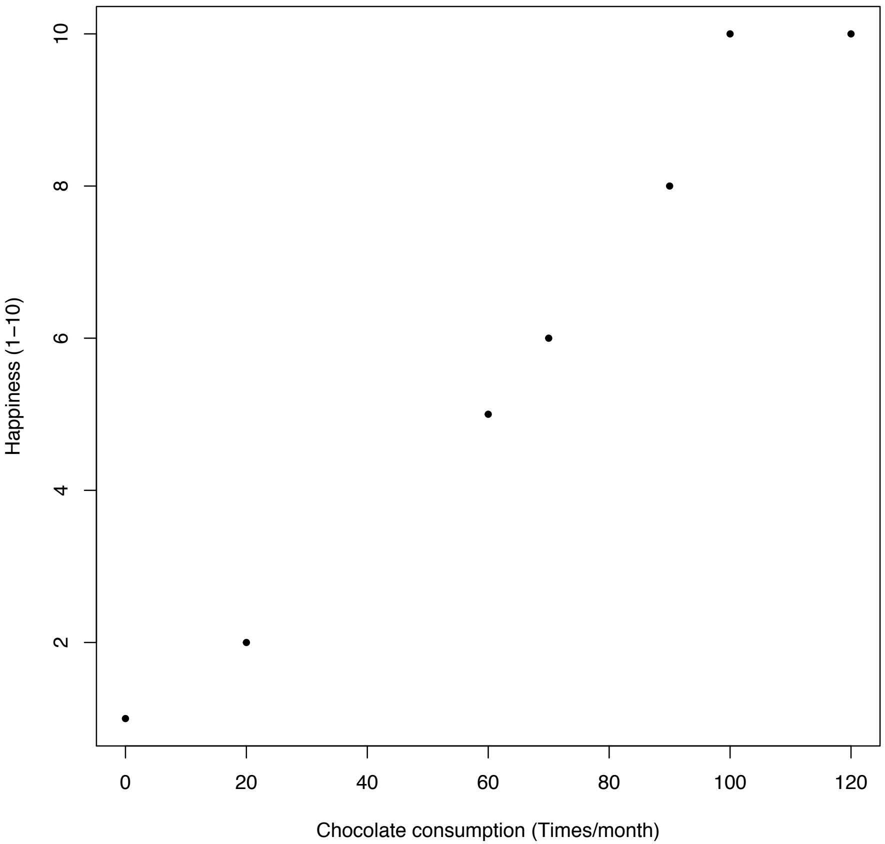
We are often interested in the statistical dependence between two variables, aka "correlation"

Pearson correlation

- Is a measure of linear association
- Pearson correlation coefficient (r) indicates the strength of a <u>linear</u> relationship between two variables
- Pearson correlation coefficient (r) is defined as the average value of the product

  (*X* in SUs)*(*Y* in SUs)
- where SU = standard units
- *X* in SUs = (X – mean(X))/SD(X)
- *Y* in SUs = (Y – mean(Y))/SD(Y)


Happiness (1−10)
2
4
6
8
10
0
20
40
60
80
100
120
Chocolate consumption (Times/month)



Happiness	Chocolate consumption
6	70
5	60
1	0
8	90
2	20
10	100
10	120

Pearson correlation

Average of (*X* in SUs)*(*Y* in SUs)

- where SU = standard units
- *X* in SUs = (X – mean(X))/SD(X)
- *Y* in SUs = (Y – mean(Y))/SD(Y)

- X = (6,5,1,8,2,10,10), mean(X) = 6, SD(X)= 3.605551
- X in SUs = (0.0000000 ,-0.2773501, -1.3867505, 0.5547002, -1.1094004, 1.1094004, 1.1094004)
- Y=(70,60,0,90,20,100,120), mean(Y) = 65.71429, SD(Y) = 43.14979
- Y in SUs = (0.09932178, -0.13242904, -1.52293392, 0.56282341, -1.05943229, 0.79457422, 1.25807585)
- Average of (*X* in SUs)*(*Y* in SUs) = 5.913401/6 = 0.9855668

Pearson correlation-Guide for interpretation

Evans, J. D. (1996) (Straightforward statistics for the behavioral sciences.) suggests for the absolute value of r:

.00-.19 “very weak”
.20-.39 “weak”
.40-.59 “moderate”
.60-.79 “strong”
.80-1.0 “very strong”

Pearson correlation

$$-1 \leq r \leq 1$$

r* is a *unit-less quantity

the closer r is to –1 or 1, the more tightly the points on the scatterplot are clustered around a line

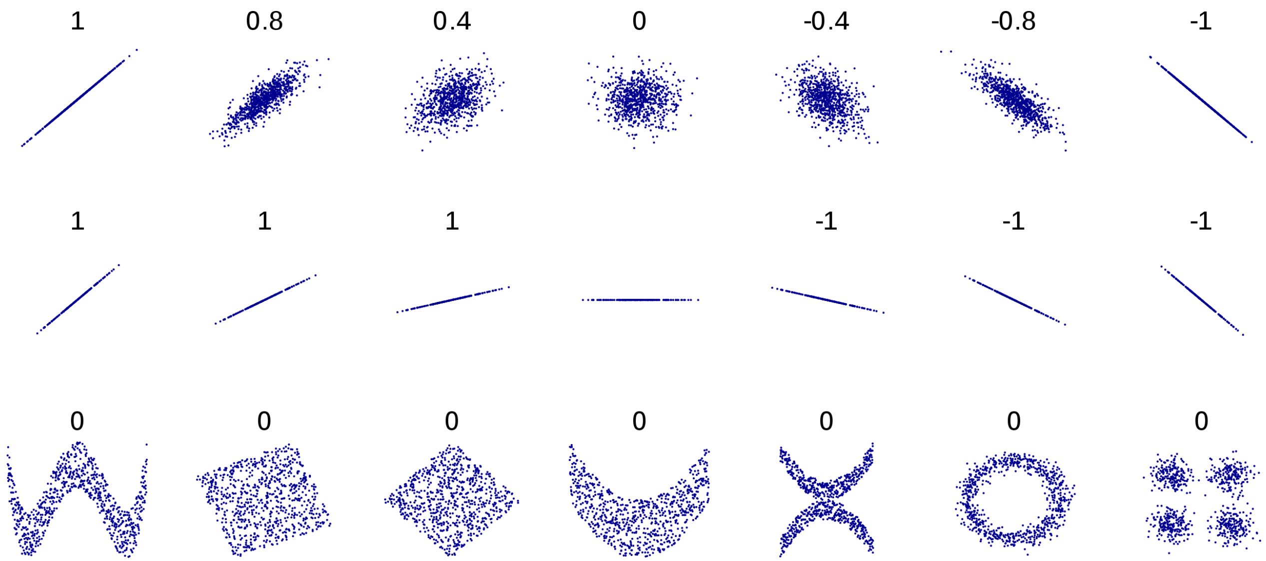


Image source: Wikipedia

To recap …

- ***r is*** **a measure of *LINEAR ASSOCIATION***
- ***r*** **does *NOT* tell us if *Y* is a function of *X***
- ***r*** **does *NOT* tell us if *X causes Y***
- ***r*** **does *NOT* tell us if *Y causes X***
- ***r*** **does *NOT* tell us the slope of the line (except for its sign)**
- ***r*** **does *NOT* tell us what the scatterplot looks like (it is only a summary of the data)**

CORRELATION IS NOT CAUSATION

- You *cannot* infer that since *X* and *Y* are highly correlated (r close to –1 or 1), *X* is *causing* a change in *Y*
- *Y* could be causing *X*
- *X* and *Y* could both be varying along with a third, possibly unknown variable (either causal or not)

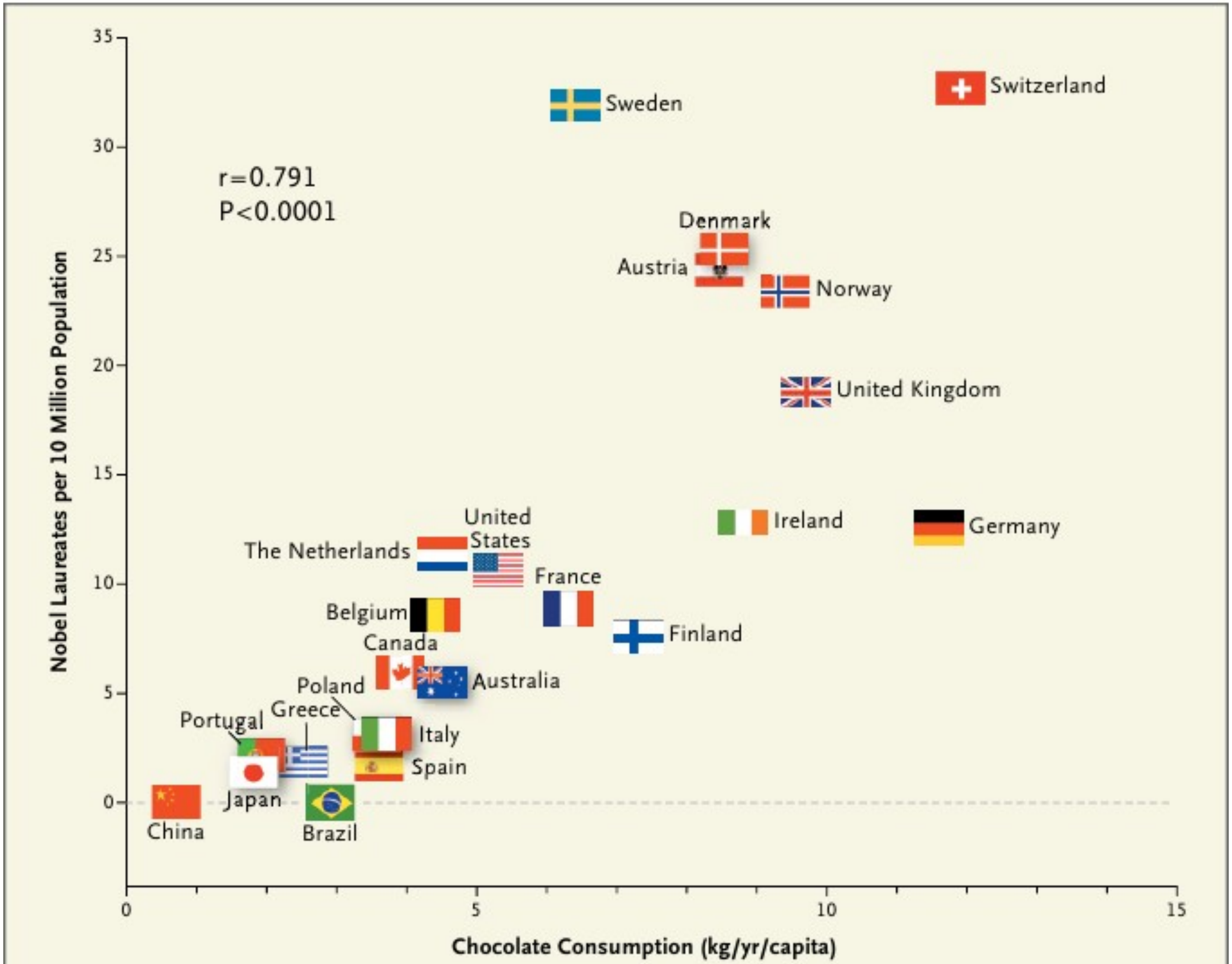
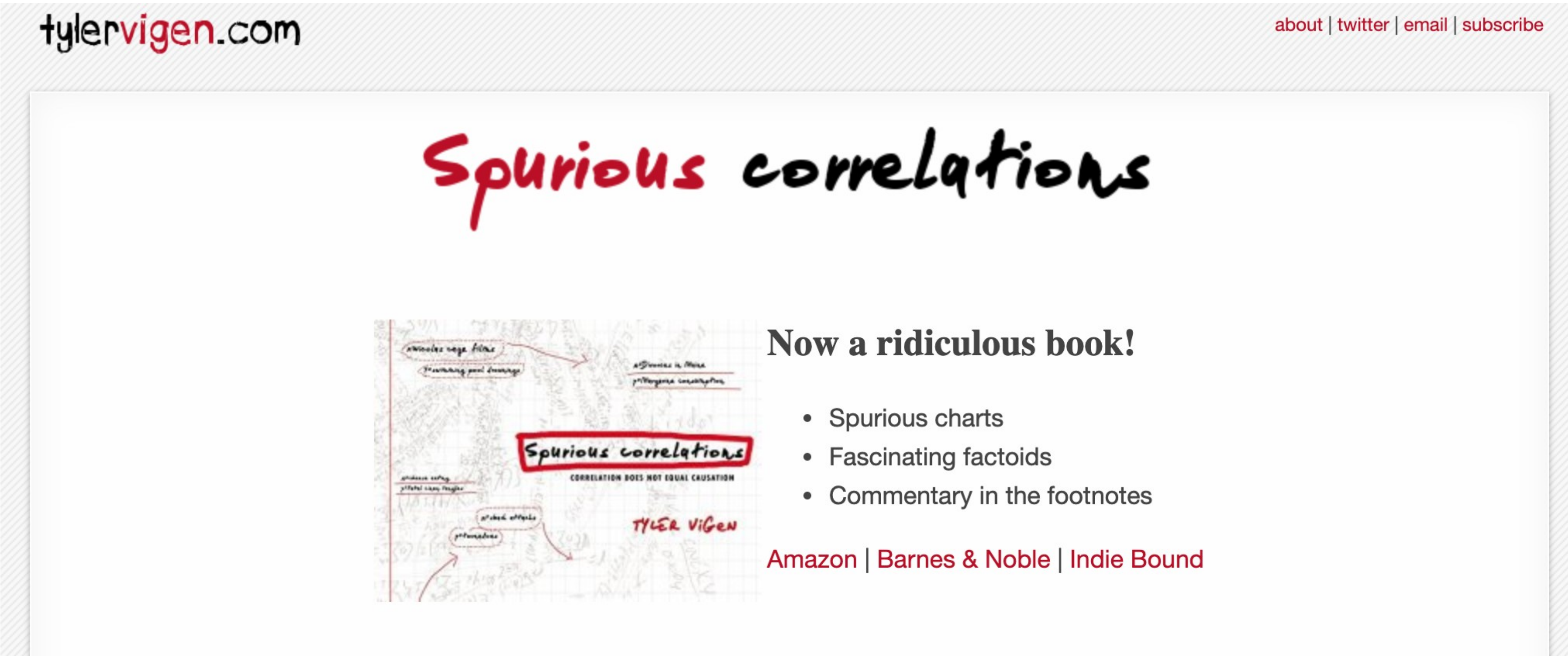


Figure 1. **Correlation between Countries' Annual Per Capita Chocolate Consumption and the Number of Nobel Laureates per 10 Million Population.**

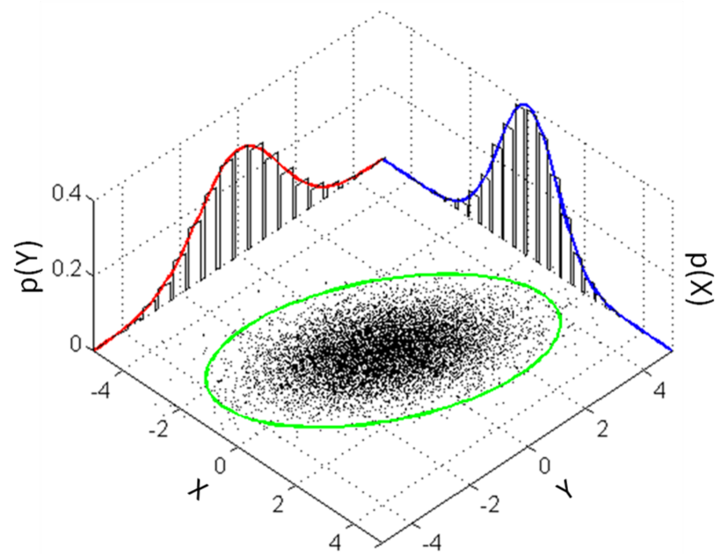
Source: https://www.nejm.org/doi/full/10.1056/NEJMon1211064

CORRELATION IS NOT CAUSATION



Assumptions of Pearson correlation

- The only assumption of Pearson correlation is that the data follows a bivariate normal distribution

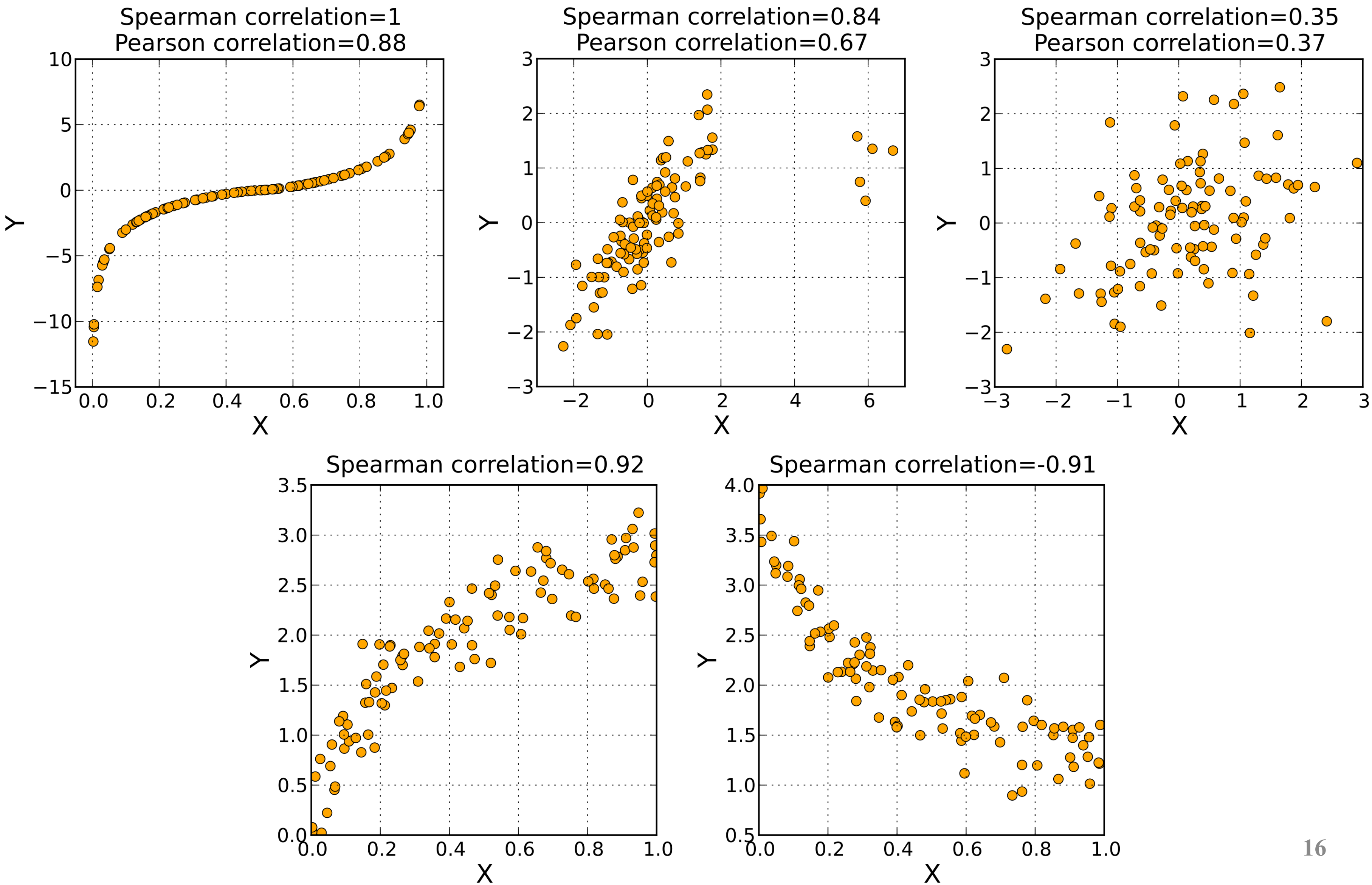


- When this assumption is not met, alternative measures of association between two variables should be used
  - Spearman rank correlation
  - Kendal rank correlation

Spearman (rank) correlation

- A nonparametric measure of rank correlation
- The Spearman correlation coefficient (denoted by the Greek letter rho) is defined as the Pearson correlation coefficient between the rank variables
  – also a unit-less value varying between -1 and +1
- It tells us how well the relationship between two variables can be described using a monotonic function
  – increase/decrease in one variable is associated with increase/decrease in the other variable
  – Not necessarily linear association!

Spearman correlation



In R:

```
>?cor

>?cor.test
```

```
>cor(x,y)

>cor.test(x,y)
```

- Note, however, that if there are *missing values (NA)*, then you will get an *error message*
- Elementary statistical functions in R require *no* missing values, or explicit statement of what to do with *NA* *(na.rm=TRUE)*

```
> cor.test(x,y)

    Pearson's product-moment correlation

data:  x and y
t = 21.5241, df = 98, p-value < 2.2e-16
alternative hypothesis: true correlation is not equal to 0
95 percent confidence interval:
 0.8667723 0.9376171
sample estimates:
      cor
0.9085158
```

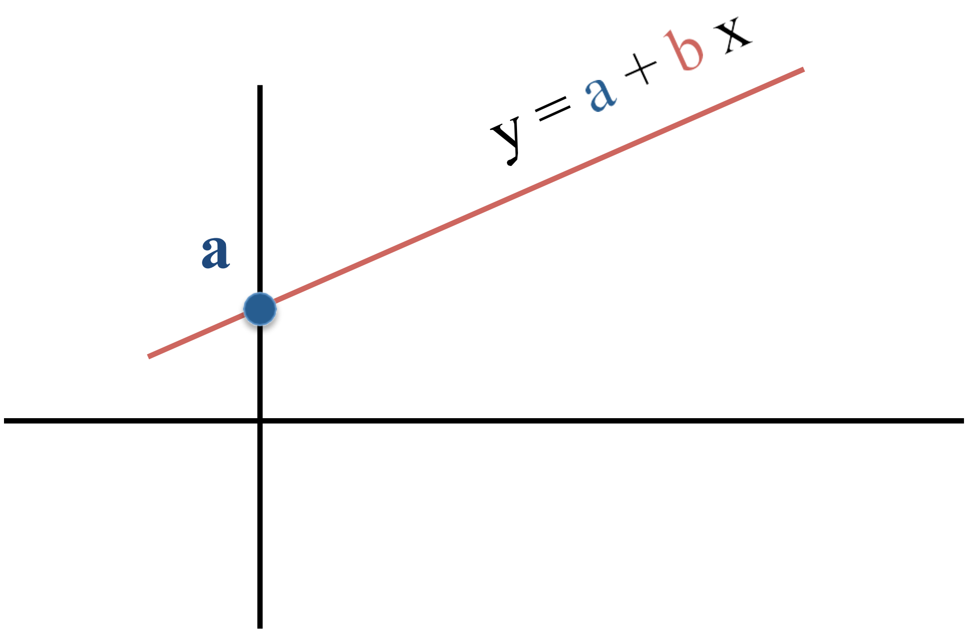
- **Correlation** describes the association between variables, but does not describe it

- Often it is useful to obtain a mathematical model that describes the association between variables, hence **regression**

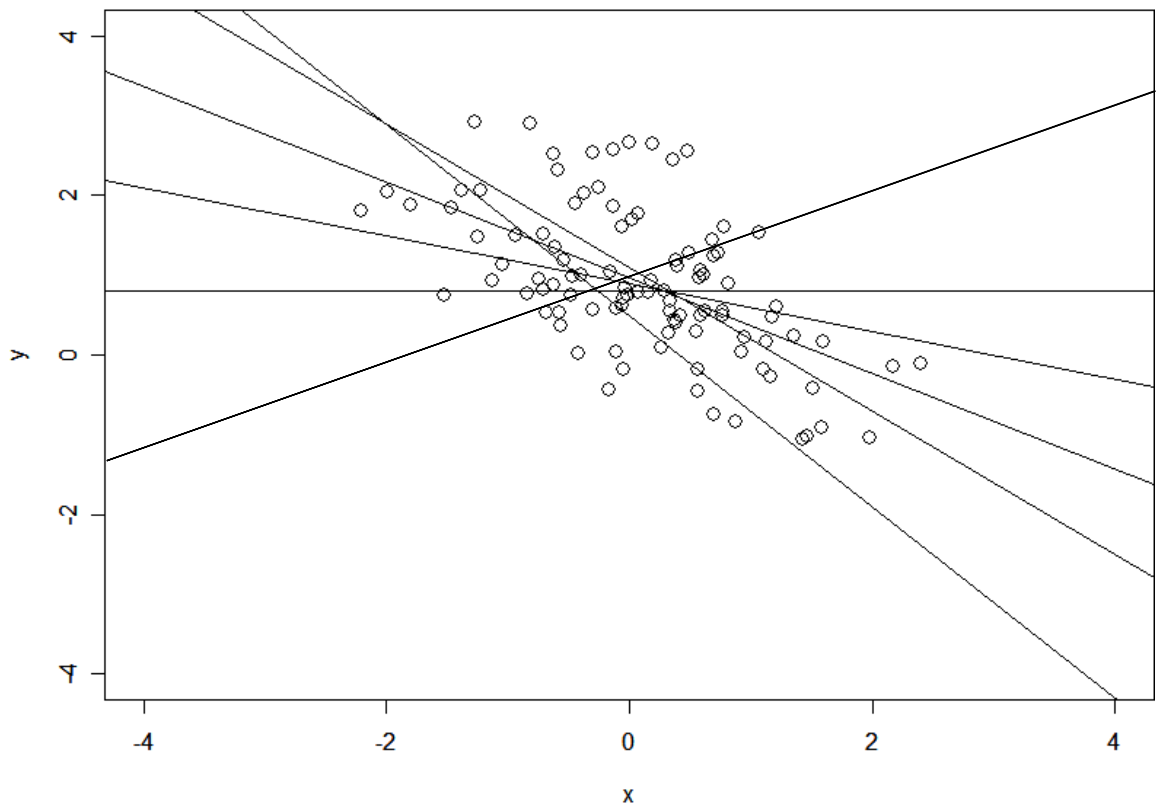
The equation for a line that can be used to predict y knowing x (in slope-intercept form) looks like

$$y = a + b\,x$$

where *a* is called the *intercept* and *b* is the *slope*.



What is the “best” line that fits this data ? → need a criteria
Can we use it to summarize the relation between x and y ?



$y = 0.9 + 0.6x$

$y = 0.8 + 0x$

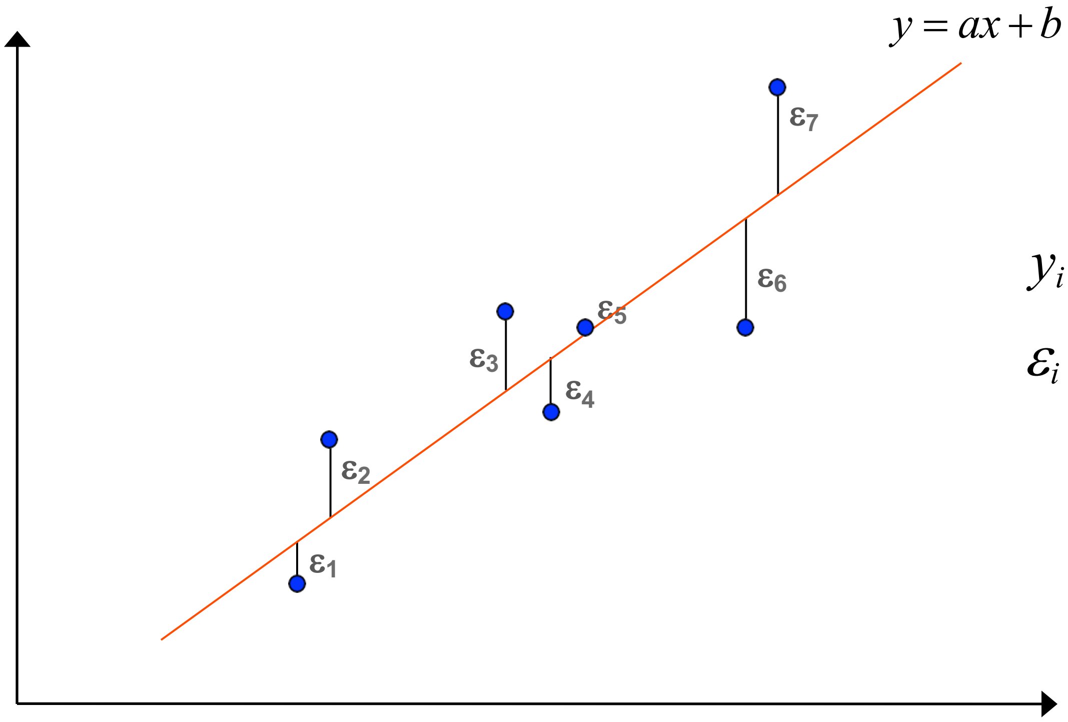
$y = 0.9 – 0.3x$

$y = 1 – 0.6x$

$y = 1.1 – 0.9x$

$y = 0.5 – 1.2x$

Least-squares approach to fit a line



$$y_i = ax_i + b + \varepsilon_i$$

$$\varepsilon_i = y_i - (ax_i + b)$$

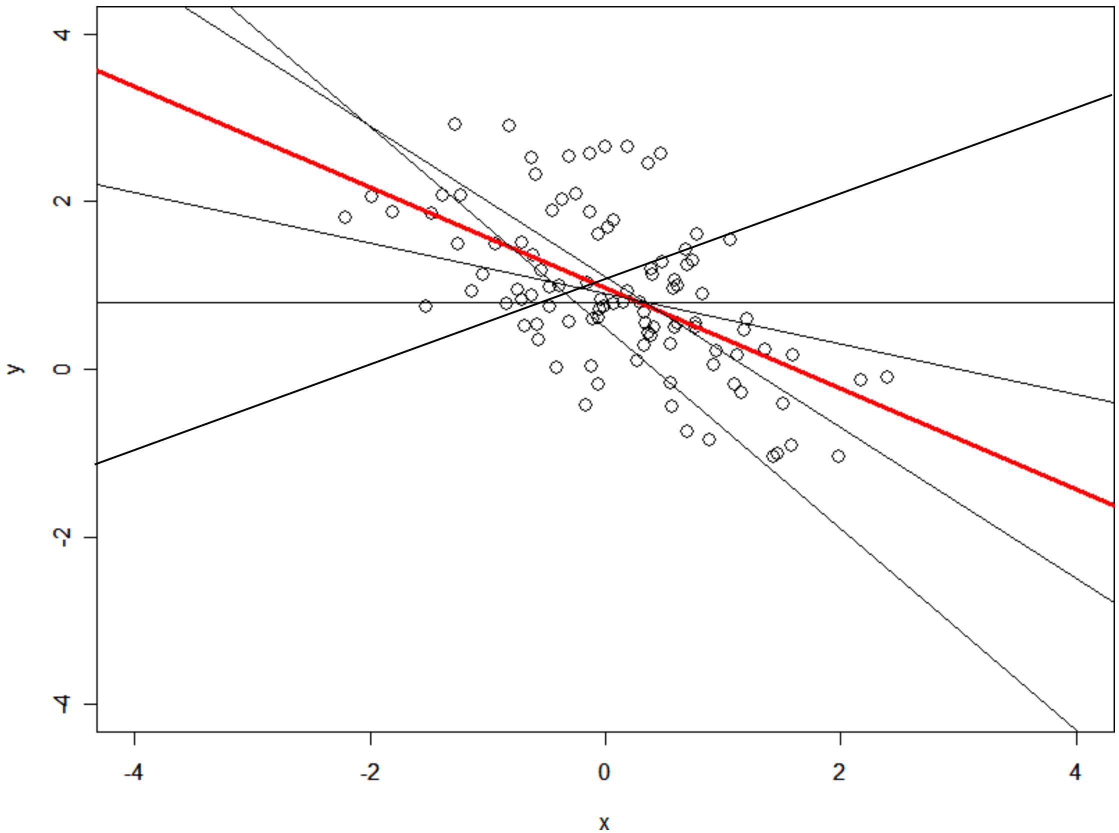
The least-squares procedure finds the straight line with the smallest sum of squares of vertical errors.

Finds a regression line such that $\sum_i \varepsilon_i^2 = \varepsilon_1^2 + \varepsilon_2^2 + \varepsilon_3^2 + \ldots$ is minimum.

Over all possible straight lines,

$y = 1 - 0.6x$ is the "best" possible line

according to least-squares criterion



$y = 0.9 + 0.6x$

$y = 0.8 + 0x$

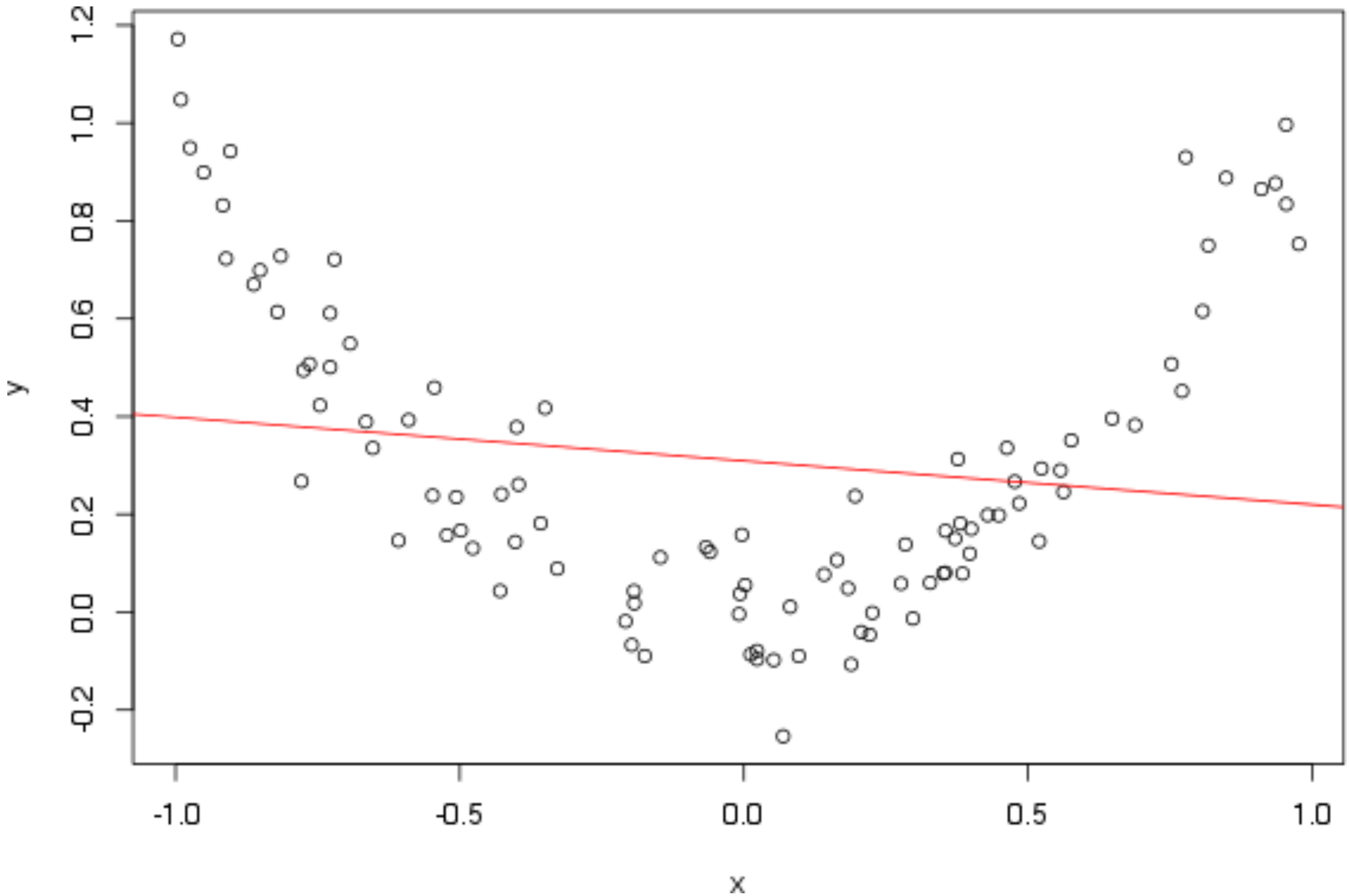
$y = 0.9 – 0.3x$

$y = 1 – 0.6x$

$y = 1.1 – 0.9x$

$y = 0.5 – 1.2x$

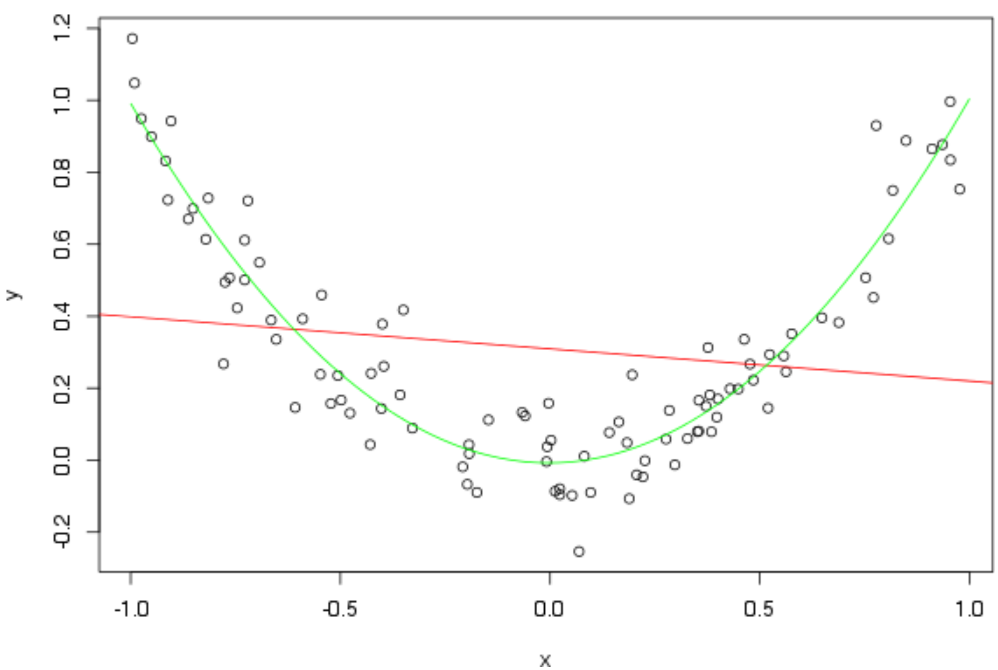
What if the association is not linear ?



What if the data is not linear ?

Use a polynomial regression

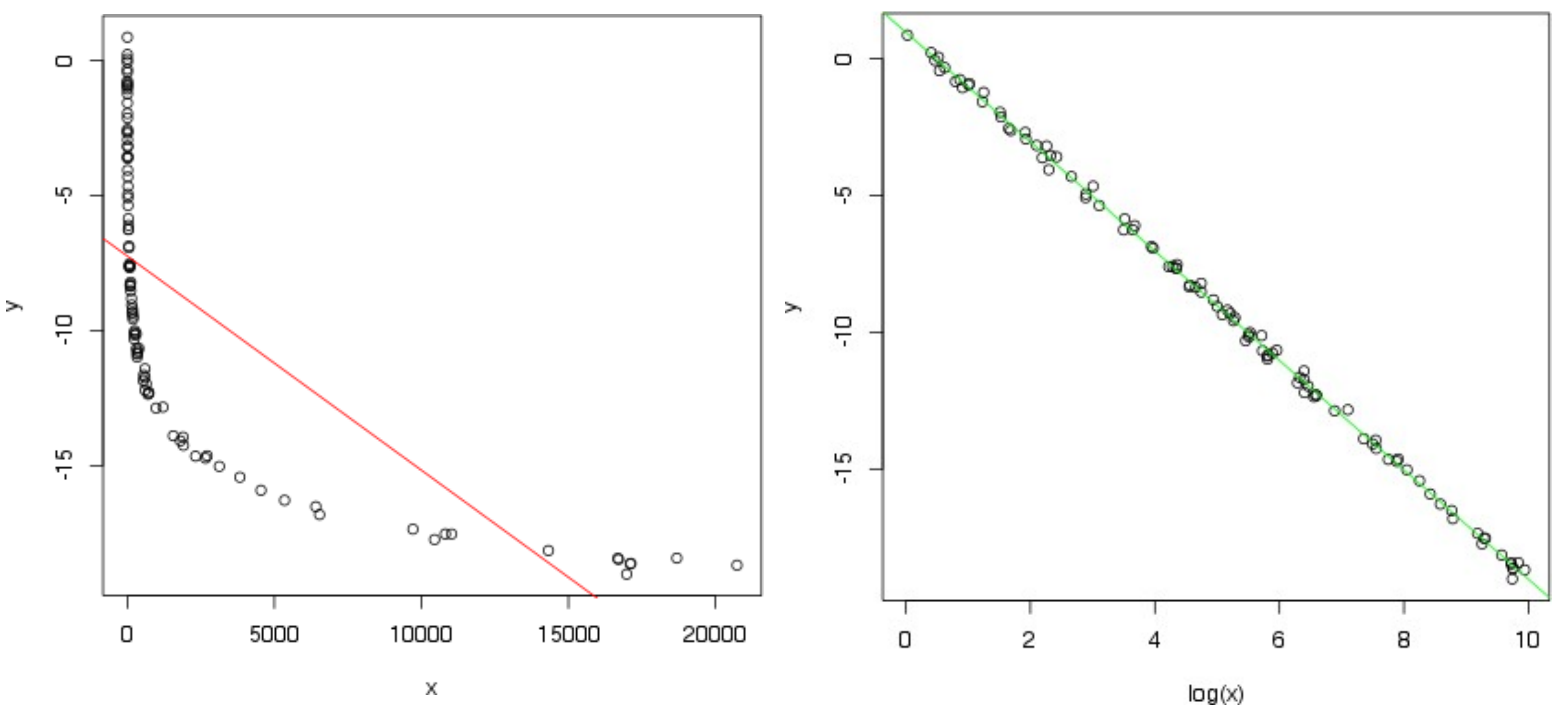
$$y = b_0 + b_1 x + b_2 x^2$$



What if the association is not linear ?

Consider transforming the data (log)

$$\log(y) = a + b\,x$$



Linear models in matrix form

$$Y_i = \beta_0 + \beta_1 X_{\mathbf{i1}} + \varepsilon_i$$

is equivalent to

$$\begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{bmatrix} = \begin{bmatrix} 1 & X_1 \\ 1 & X_2 \\ 1 & \vdots \\ 1 & X_n \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} + \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_n \end{bmatrix}$$

or $$\mathbf{Y} = \mathbf{X\beta} + \boldsymbol{\varepsilon}$$

Linear models in matrix form

$$Y_i = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \varepsilon_i$$

is equivalent to

$$\begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{bmatrix} = \begin{bmatrix} 1 & X_{11} & X_{12} \\ 1 & X_{21} & X_{22} \\ 1 & \vdots & \vdots \\ 1 & X_{n1} & X_{n2} \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_{p-1} \end{bmatrix} + \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_n \end{bmatrix}$$

or $\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}$

Linear models in matrix form

$$Y_i = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \ldots + \beta_{p-1} X_{ip-1} + \varepsilon_i$$

is equivalent to

$$\begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{bmatrix} = \begin{bmatrix} 1 & X_{11} & X_{12} & \cdots & X_{1p-1} \\ 1 & X_{21} & X_{22} & \cdots & X_{2p-1} \\ 1 & \vdots & \vdots & \ddots & \vdots \\ 1 & X_{n1} & X_{n2} & \cdots & X_{np-1} \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_{p-1} \end{bmatrix} + \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_n \end{bmatrix}$$

or $$\mathbf{Y} = \mathbf{X\beta} + \boldsymbol{\varepsilon}$$

Linear models in matrix form

$$Y_i = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \ldots + \beta_{p-1} X_{ip-1} + \varepsilon_i$$

is equivalent to

$$\begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{bmatrix} = \begin{bmatrix} 1 & X_{11} & X_{12} & \cdots & X_{1p-1} \\ 1 & X_{21} & X_{22} & \cdots & X_{2p-1} \\ 1 & \vdots & \vdots & \ddots & \vdots \\ 1 & X_{n1} & X_{n2} & \cdots & X_{np-1} \end{bmatrix} \boxed{\begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_{p-1} \end{bmatrix}} + \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_n \end{bmatrix}$$

or $\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}$

Least-square estimation of regression coefficients

Least-square estimation of regression coefficients

$\mathbf{b} = (b_0 \ldots b_{p-1})'$ estimator of $\boldsymbol{\beta}$ is computed as follows:

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}$$

$$\mathbf{X}'\mathbf{X}\boldsymbol{\beta} = \mathbf{X}'\mathbf{Y} \qquad \textbf{where} \quad E\{\boldsymbol{\varepsilon}\} = \mathbf{0}$$

Least-square estimation of regression coefficients

$\mathbf{b} = (b_0 \ldots b_{p-1})'$ estimator of $\boldsymbol{\beta}$ is computed as follows:

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}$$

$$\mathbf{X'X}\boldsymbol{\beta} = \mathbf{X'Y} \qquad \textbf{where} \quad E\{\boldsymbol{\varepsilon}\} = \mathbf{0}$$

$$\boldsymbol{\beta} = (\mathbf{X'X})^{-1}\mathbf{X'Y}$$

Computationally intensive

$$Y = b_0 + b_1 x_1 + b_2 x_2 + b_3 x_3$$

in R:

```
yvar ~ xvar1 + xvar2 + xvar3
```

read "~" as "described (or modeled) by"

By default, an intercept is included in the model

To leave the intercept out:

```
yvar ~ -1 + xvar1 + xvar2 + xvar3
```

$$Y = b_0 + b_1 x_1 + b_2 x_2 + b_3 x_3$$

in R:

```
yvar ~ xvar1 + xvar2 + xvar3
```

read "~" as "described (or modeled) by"

By default, an intercept is included in the model

To leave the intercept out:

```
yvar ~ -1 + xvar1 + xvar2 + xvar3
yvar ~ 0 + xvar1 + xvar2 + xvar3
```

Generic form

`response ~ predictors`

predictors can be `numeric` or `categorical`

R symbols to create formulas

- `+` to *add* more variables
- `-` to *leave out* variables
- `:` to introduce *interactions* between two terms
- `*` to include *both interactions and the terms*

  (`a*b` is the same as `a + b + a:b`)
- `^n` *adds all terms* including interactions up to order n
- `I()` treats what's in () as a *mathematical expression*

Let’s walk through an example in R

Using the CLASS dataset, from the program SAS
(units have been modified from imperial to metric)

The CLASS dataset from SAS

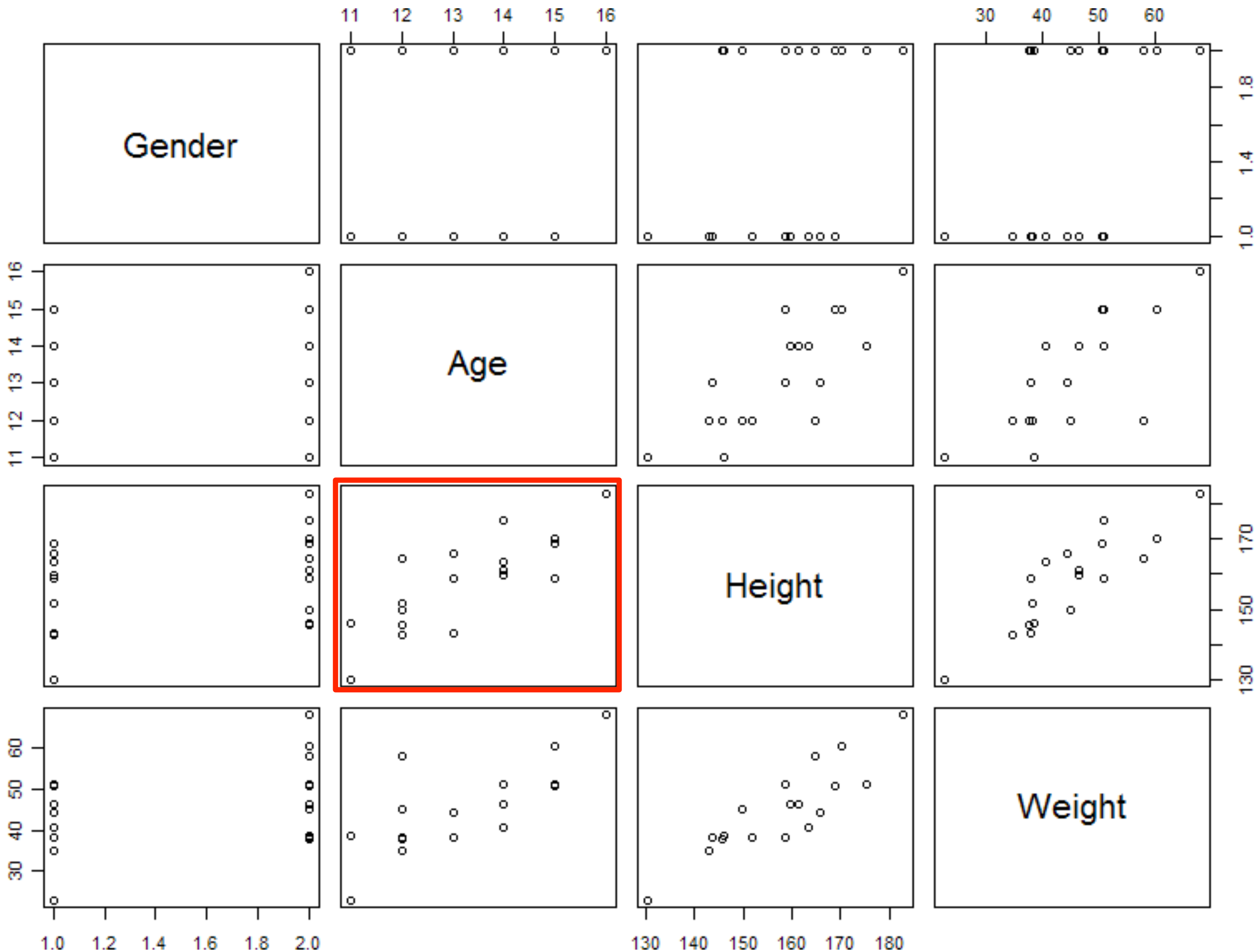
```
> class
      Name Gender Age  Height  Weight
1    JOYCE      F  11 130.302 22.8765
2   THOMAS      M  11 146.050 38.5050
3    JAMES      M  12 145.542 37.5990
4     JANE      F  12 151.892 38.2785
5     JOHN      M  12 149.860 45.0735
6   LOUISE      F  12 143.002 34.8810
7   ROBERT      M  12 164.592 57.9840
8    ALICE      F  13 143.510 38.0520
9  BARBARA      F  13 165.862 44.3940
10 JEFFREY      M  13 158.750 38.0520
11   CAROL      F  14 159.512 46.4325
12   HENRY      M  14 161.290 46.4325
13  ALFRED      M  14 175.260 50.9625
14    JUDY      F  14 163.322 40.7700
15   JANET      F  15 158.750 50.9625
16    MARY      F  15 168.910 50.7360
17  RONALD      M  15 170.180 60.2490
18 WILLIAM      M  15 168.910 50.7360
19  PHILIP      M  16 182.880 67.9500
```

The CLASS dataset from SAS

```
> summary(class[,-1])

Gender      Age              Height           Weight
F: 9   Min.   :11.00   Min.   :130.3   Min.   :22.88
M:10   1st Qu.:12.00   1st Qu.:148.0   1st Qu.:38.17
       Median :13.00   Median :159.5   Median :45.07
       Mean   :13.32   Mean   :158.3   Mean   :45.31
       3rd Qu.:14.50   3rd Qu.:167.4   3rd Qu.:50.85
       Max.   :16.00   Max.   :182.9   Max.   :67.95


> pairs(class[,-1])
```


Gender
Age
Height
Weight
11 12 13 14 15 16
30 40 50 60
1.0 1.4 1.8
11 12 13 14 15 16
130 150 170
30 40 50 60
1.0 1.2 1.4 1.6 1.8 2.0
130 140 150 160 170 180

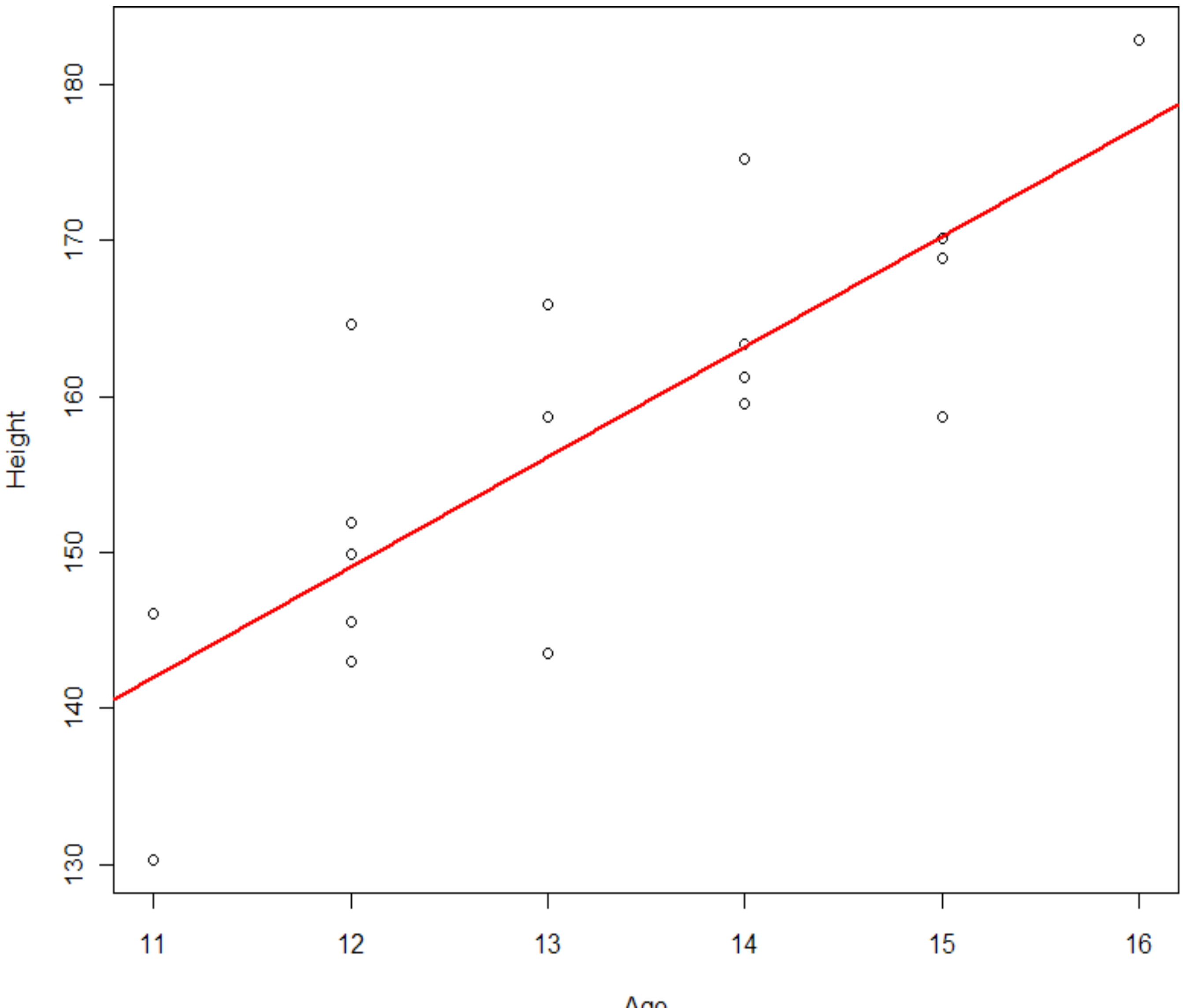
```
> model <- lm( Height ~ Age, data=class)
> model

Call:
lm(formula = Height ~ Age, data = class)

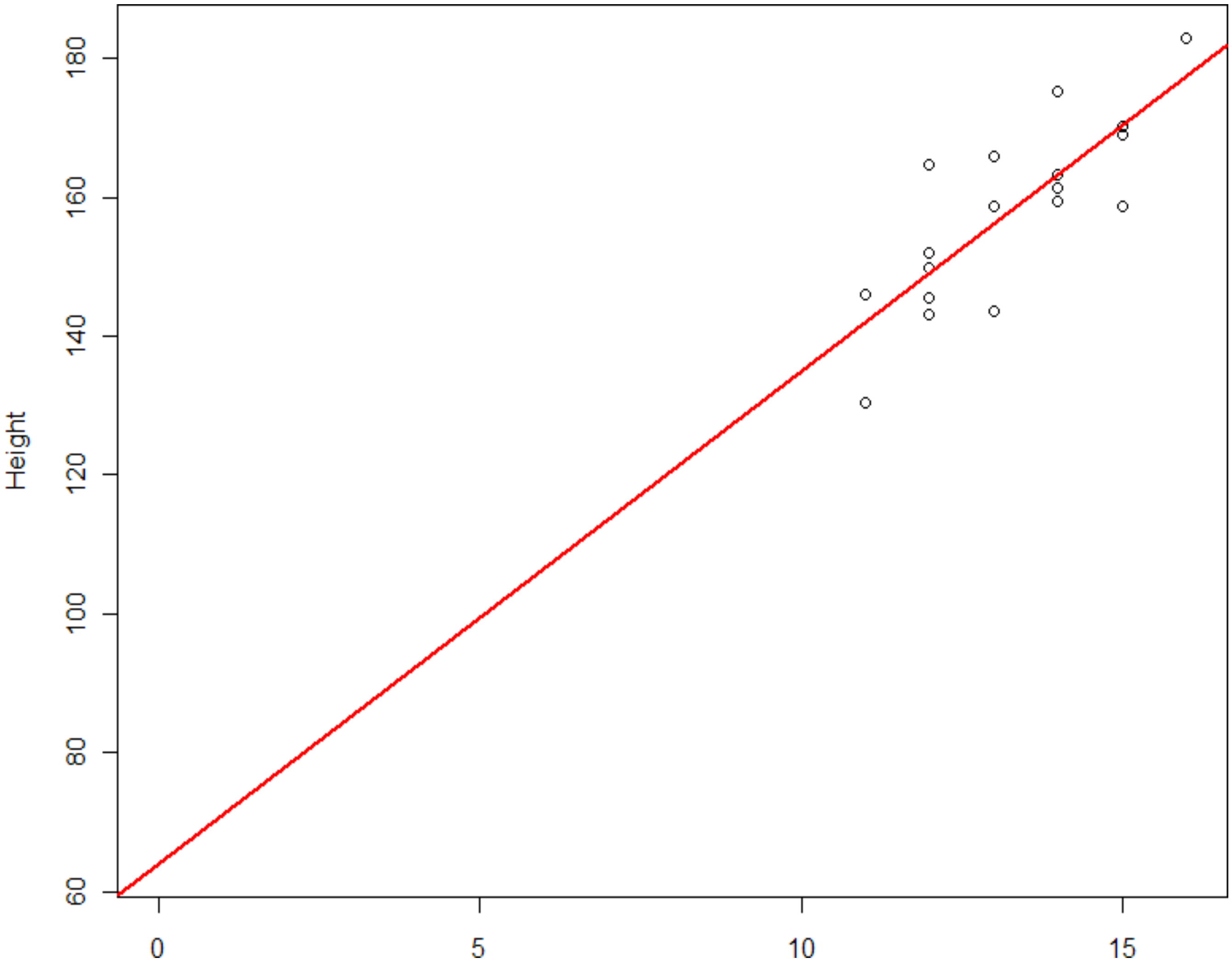
Coefficients:
(Intercept)          Age
      64.07         7.08
```

Model: Height = 64.07 + 7.08 x Age

```
> plot( class$Age, class$Height)
> abline(model, col="red", lwd=2)
```



```
> plot(class$Age, class$Height,
  xlim=range(0,Age),
  ylim=range(coef(model)[1], Height))
> abline(model, col="red", lwd=2)
```



Example of summary results of the `lm` command in R

```
> summary( lm( Height ~ Age, data = class) )

Call:
lm(formula = Height ~ Age)

Residuals:
      Min          1Q    Median          3Q        Max
-12.59000  -3.57300  -0.07867   3.49000  15.57133

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)   64.069     16.565   3.868  0.00124 **
Age            7.079      1.237   5.724 2.48e-05 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 7.832 on 17 degrees of freedom
Multiple R-squared: 0.6584,     Adjusted R-squared: 0.6383
F-statistic: 32.77 on 1 and 17 DF,  p-value: 2.48e-05
```

Example of summary results of the `lm` command in R

```
> summary( lm( Height ~ Age) )
```

Function call

```
Call:
lm(formula = Height ~ Age)

Residuals:
      Min          1Q     Median          3Q         Max
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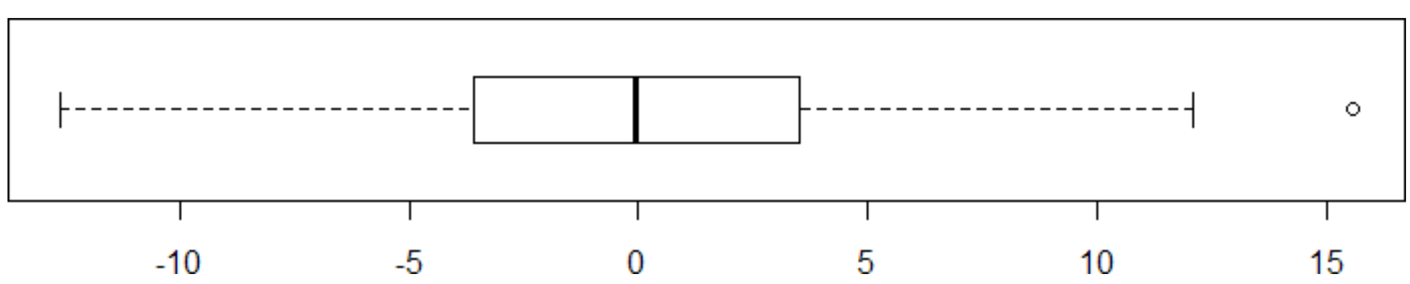
F-statistic: 32.77 on 1 and 17 DF,  p-value: 2.48e-05
```

Five-number summary of the residuals (but no mean – why ?), equivalent to

```
> fivenum( residuals( model ) )
       8       11       17        4        7
 -12.590   -3.573   -0.078    3.490   15.571
```

or, graphically, using a boxplot:

```
> boxplot( residuals ( model), horizontal=T)
```



Example of summary results of the `lm` command in R

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F-statistic: 32.77 on 1 and 17 DF,  p-value: 2.48e-05
```

Coefficients

These statistical tests tell us if the parameters are significantly different from 0.

****It is not interesting for the intercept, but usually interesting for the slope.**

Estimate and Std. Error are used for hypothesis testing

T-value = Estimate / Std. Error

This assumes that the residuals follow a normal distribution!

Example of summary results of the `lm` command in R

```
> summary( lm( Height ~ Age) )

Call:
lm(formula = Height ~ Age)

Residuals:
      Min        1Q    Median        3Q       Max
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Age            7.079      1.237   5.724 2.48e-05 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

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Multiple R-squared: 0.6584,     Adjusted R-squared: 0.6383
F-statistic: 32.77 on 1 and 17 DF,  p-value: 2.48e-05
```

RSE (Residual Standard Error) and degrees of freedom

The number of *degrees of freedom* indicates the number of independant pieces of data that are available to estimate the error

While we have 19 residuals here, they are not all independent: for example, the last one is constrained because the sum of all residuals must be 0.

The number of DF

total observations – number of parameters estimated

Two parameters are estimated (intercept + coefficient), so 19-2 = 17

Example of summary results of the `lm` command in R

```
> summary( lm( Height ~ Age) )

Call:
lm(formula = Height ~ Age)

Residuals:
      Min         1Q     Median         3Q        Max
-12.59000  -3.57300  -0.07867    3.49000  15.57133

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)   64.069     16.565   3.868  0.00124 **
Age            7.079      1.237   5.724 2.48e-05 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 7.832 on 17 degrees of freedom
Multiple R-squared: 0.6584,     Adjusted R-squared: 0.6383
F-statistic: 32.77 on 1 and 17 DF,  p-value: 2.48e-05
```

RSE (Residual Standard Error) and degrees of freedom

The residual standard error is the standard deviation of the residuals (which we would usually like to be small)

It is not exactly equal to what the sd command would return:

```
> sd(residuals(model))
[1] 7.611075
> sqrt(sum(residuals(model)^2)/18)
[1] 7.611075
```

Here, we must divide by the number of degrees of freedom to get the same number:

```
> sqrt(sum(residuals(model)^2)/17)
[1] 7.831732
```

Example of summary results of the `lm` command in R

```
> summary( lm( Height ~ Age) )

Call:
lm(formula = Height ~ Age)

Residuals:
      Min        1Q    Median        3Q       Max
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Multiple and adjusted R-squared

R^2 is the proportion of the total variance in the response data that is explained by the model

if R^2=1, the data fits perfectly on a straight line, and the model explains all the variance

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```
>summary(model)$r.squared
[1] 0.6584257
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[1] 0.6584257
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```
>summary(model)$r.squared
[1] 0.6584257
>cor(Age, Height)^2
[1] 0.6584257
```

The Adjusted R-squared is similar to R-squared, but it takes into account the number of variables in the model (we will come back to this later).

Example of summary results of the `lm` command in R

```
> summary( lm( Height ~ Age) )

Call:
lm(formula = Height ~ Age)

Residuals:
      Min        1Q    Median        3Q       Max
-12.59000  -3.57300  -0.07867   3.49000  15.57133

Coefficients:
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```

F-test for significance of regression

The F-statistic allows us to test if the whole regression (adding all variables *vs* having only the intercept in) is significant.

It calculates the F value which is given by the variation explained by our model divided by the variation that remains.

Mathematically : $$\frac{\text{SS(mean)-SS(fit)/(pfit-pmean)}}{\text{SS(fit)/(n-pfit)}}$$

Pfit= number of parameters in the fit (2 parameters)
Pmean = number of parameters in the mean line (1 parameter)
Note: With only one variable, it provides *exactly* the same result as the t-test for the significance of the coefficient of this variable.

Challenge

Investigate the correlation and the relationship between weight and height using R basic commands

Multiple regression:
assessing the effect of several variables *together*

What happens if both,
age and weight variables
were included in the same model ?

One multiple regression with two variables

```
Call:
lm(formula = Height ~ Age + Weight)

Residuals:
     Min       1Q   Median       3Q      Max 
-9.20695 -3.30604 -0.04478  2.11432 10.41880 

Coefficients:
            Estimate Std. Error t value Pr(>|t|)    
(Intercept) 81.77355   12.90896   6.335 9.92e-06 ***
Age          3.11575    1.34668   2.314  0.03431 *  
Weight       0.35064    0.08827   3.973  0.00109 ** 
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1 

Residual standard error: 5.728 on 16 degrees of freedom
Multiple R-squared: 0.828,      Adjusted R-squared: 0.8065 
F-statistic: 38.52 on 2 and 16 DF,  p-value: 7.646e-07
```

This model allows us to determine the respective contribution of each variable separately.

```
Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) 81.77355   12.90896   6.335 9.92e-06 ***
Age          3.11575    1.34668   2.314  0.03431 *
Weight       0.35064    0.08827   3.973  0.00109 **
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

This is similar to the simple regression case.

Each test is conducted assuming that the tested parameter is the last one entering the model:

« If *weight* is already in the model, is the coefficient for *age* significantly different from 0 ? »

Two single regressions vs one multiple regression

```
Coefficients:
             Estimate Std. Error t value Pr(>|t|)    
(Intercept)    64.069     16.565   3.868  0.00124 ** 
Age             7.079      1.237   5.724 2.48e-05 ***
```

```
Coefficients:
             Estimate Std. Error t value Pr(>|t|)    
(Intercept) 108.12816    6.80692  15.885 1.24e-11 ***
Weight        0.50194    0.06644   7.555 7.89e-07 ***
```

```
Coefficients:
             Estimate Std. Error t value Pr(>|t|)    
(Intercept)  81.77355   12.90896   6.335 9.92e-06 ***
Age           3.11575    1.34668   2.314  0.03431 *  
Weight        0.35064    0.08827   3.973  0.00109 ** 
```

While both age and weight seem significant by themselves, age is much less significant when weight is already included (see also the R^2).

It is likely that a lot of the information provided by the age is also provided by the weight, so that there may be little need to have both terms in the model.

```
Multiple R-squared: 0.828,      Adjusted R-squared: 0.8065
```

As before, R^2 is the proportion of the total variance in the response data that is explained by the model.

Adding a new variable in the model will always increase R^2, up to 1 when there the number of degrees of freedom is 0 (number of parameters to estimate = number of observations).

Multiple and adjusted R-squared

```
Multiple R-squared: 0.828,      Adjusted R-squared: 0.8065
```

The adjusted R-squared adjusts for the number of variables in the model, and does not necessarily increase when the number of variables increase; it can even be negative.

It is always equal or below R^2.

Example

```
y <- rnorm(10)
x1 <- rnorm(10); x2 <- rnorm(10); … ; x9 <-
rnorm(10)
summary(lm(y ~ x1)); summary(lm(y ~ x1+x2));
```

```
1: Multiple R-squared: 0.1419,    Adjusted R-squared: 0.03464
2: Multiple R-squared: 0.5173,    Adjusted R-squared: 0.3794
3: Multiple R-squared: 0.557,     Adjusted R-squared: 0.3355
4: Multiple R-squared: 0.5577,    Adjusted R-squared: 0.2039
5: Multiple R-squared: 0.7953,    Adjusted R-squared: 0.5395
6: Multiple R-squared: 0.8321,    Adjusted R-squared: 0.4962
7: Multiple R-squared: 0.984,     Adjusted R-squared: 0.9281
8: Multiple R-squared: 0.9851,    Adjusted R-squared: 0.866
9: Multiple R-squared:      1,    Adjusted R-squared:   NaN
```

The last regression from the example

```
Call:
lm(formula = y ~ x1 + x2 + x3 + x4 + x5 + x6 + x7 + x8 + x9)

Residuals:
ALL 10 residuals are 0: no residual degrees of freedom!

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) -0.02693         NA      NA       NA
x1           0.53886         NA      NA       NA
x2          -0.52227         NA      NA       NA
x3           0.51881         NA      NA       NA
x4           0.74757         NA      NA       NA
x5           0.14394         NA      NA       NA
x6          -0.65387         NA      NA       NA
x7          -0.48271         NA      NA       NA
x8          -0.62487         NA      NA       NA
x9           0.23759         NA      NA       NA

Residual standard error: NaN on 0 degrees of freedom
Multiple R-squared:     1,      Adjusted R-squared:   NaN
F-statistic:   NaN on 9 and 0 DF,  p-value: NA
```

F-statistic for significance of regression

```
Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) 81.77355   12.90896   6.335 9.92e-06 ***
Age          3.11575    1.34668   2.314  0.03431 *
Weight       0.35064    0.08827   3.973  0.00109 **

F-statistic: 38.52 on 2 and 16 DF,  p-value: 7.646e-07
```

Again, the F-statistic allows us to test if the whole regression (adding all variables *vs* having only the intercept in) is significant.

If any of the tests for the individual variables is significant, the F-test will generally be significant as well.

However, even if no individual variable is significant (e.g. $p < 0.05$), the F-test can still be significant.

Categorical variables, dummy variables and contrasts

We'd like to use categorical variables in a linear model, as in:

$$\textbf{Height} = b_0 + b_1\,\textbf{Age} + b_2\,\text{« }\textbf{Gender}\text{ »} + \textbf{error}$$

Intuitively, we want to estimate a « Male » and a « Female » effect.

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$$\textbf{Height} = b_0 + b_1\,\textbf{Age} + b_2\,\text{« }\textbf{Gender}\text{ »} + \textbf{error}$$

Intuitively, we want to estimate a « Male » and a « Female » effect.

In practice, categorical variables (factors in R) are turned (by default, based on alphabetical order) into **dummy variables** of the form

$$\text{Gender} = \begin{cases} 1 \text{ if Female} \\ 2 \text{ if Male} \end{cases}$$

Example of summary results of the `lm` command in R

```
Call:
lm(formula = Height ~ Age + Gender)

Residuals:
    Min      1Q  Median      3Q     Max
-8.8462 -4.8523 -0.8102  3.3677 13.5058

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)   62.291     14.957   4.165  0.00073 ***
Age            6.928      1.117   6.202 1.27e-05 ***
GenderM        7.204      3.251   2.216  0.04152 *
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 7.061 on 16 degrees of freedom
Multiple R-squared: 0.7387,     Adjusted R-squared: 0.706
F-statistic: 22.61 on 2 and 16 DF,  p-value: 2.176e-05
```

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(Intercept)   62.291     14.957   4.165  0.00073 ***
Age            6.928      1.117   6.202 1.27e-05 ***
GenderM        7.204      3.251   2.216  0.04152 *  
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 7.061 on 16 degrees of freedom
Multiple R-squared: 0.7387,     Adjusted R-squared: 0.706 
F-statistic: 22.61 on 2 and 16 DF,  p-value: 2.176e-05
```

baseline for height among Female

Example of summary results of the `lm` command in R

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lm(formula = Height ~ Age + Gender)

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    Min      1Q  Median      3Q     Max 
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Coefficients:
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GenderM        7.204      3.251   2.216  0.04152 *  
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

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F-statistic: 22.61 on 2 and 16 DF,  p-value: 2.176e-05
```

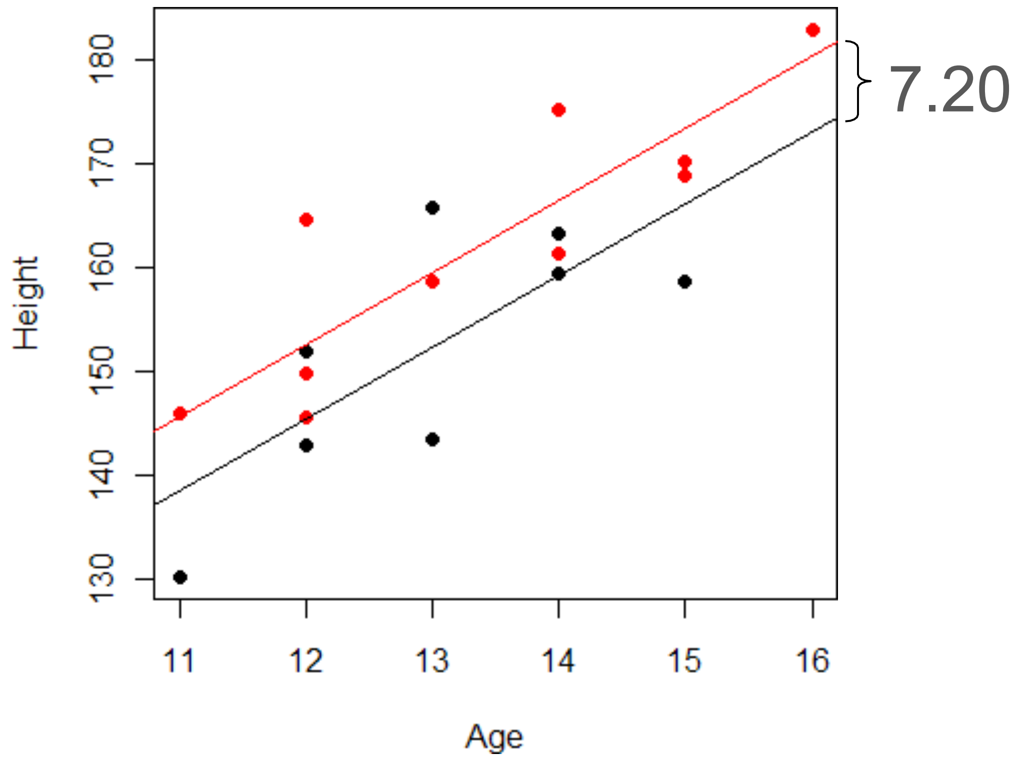
baseline for height among Female

The factor GenderM corresponds to the difference in baseline for Males compared to females.

The model specifies 2 straight lines, with the same slope but different y-intercepts:

For women: Height = 62.3 + 6.9 Age (in black)

For men: Height = 69.4 + 6.9 Age (in red)



We could also compute the difference in means between males and females directly:

```
> means <- tapply( data$Height, data$Gender, FUN=mean )
> means
       F        M
153.8958 162.3314
> diff(means)
       M
8.435622
```

This result is slightly different from the 7.20 cm difference found with the linear model.

Where does the difference come from ?

So far, we have assumed a difference between the lines, but the same slope; that is, for both men and women, the effect of age is the same.

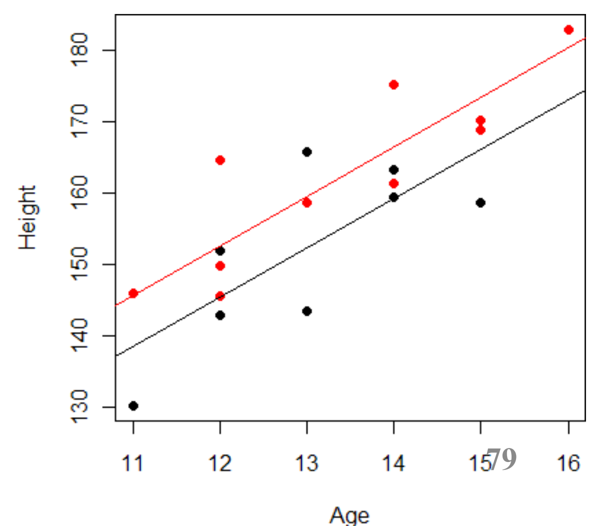
If this assumption is incorrect, it means that there is an *interaction* between the factors « age » and « gender », that is, the effect of age is different depending on the gender.

Interactions are modeled in R in the following way:

lm(formula = Height ~ Age + Gender + Age:Gender)

which is equivalent to

lm(formula = Height ~ Age * Gender)



Coefficients with an interaction

```
Call:
lm(formula = Height ~ Age * Gender)

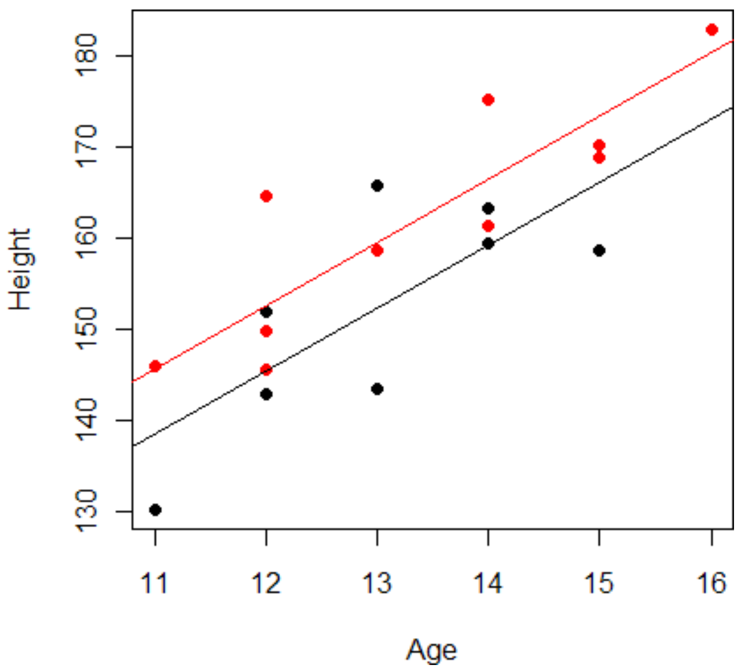
Coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept)   56.2610    24.4880   2.297  0.03640 *
Age            7.3841     1.8429   4.007  0.00114 **
GenderM       17.1304    31.5238   0.543  0.59483
Age:GenderM   -0.7468     2.3583  -0.317  0.75585
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

The coefficients can be interpreted as follows:

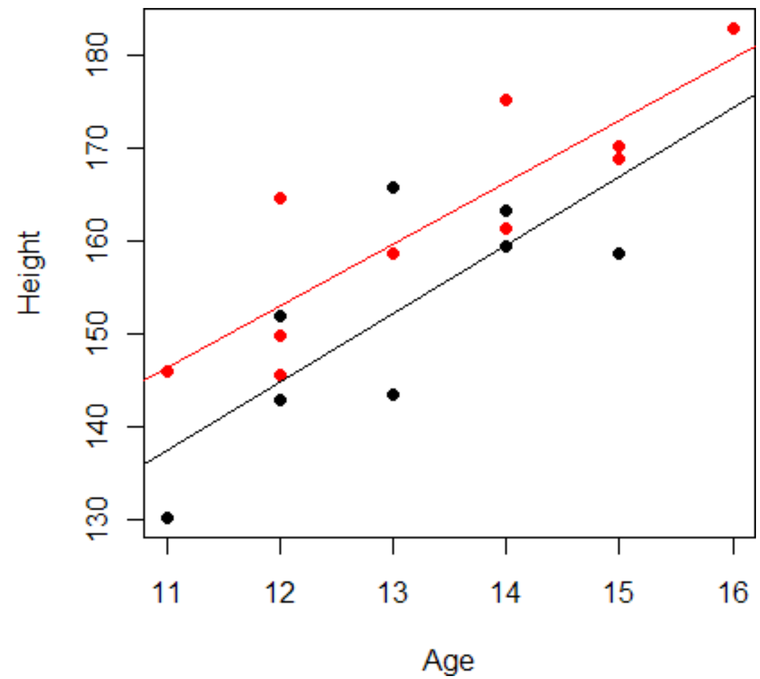
According to the model, the *height* is equal to

56.26 (the intercept)
plus 17.13, but only for males
plus 7.38 times the person's age
minus 0.75 times the person's age, but only for males.

Different slopes



No interaction



With interaction

What if Males were the baseline ?

```
Call:
lm(formula = Height ~ Age + Gender)

Residuals:
    Min      1Q  Median      3Q     Max 
-8.8462 -4.8523 -0.8102  3.3677 13.5058 

Coefficients:
            Estimate Std. Error t value Pr(>|t|)    
(Intercept)   62.291     14.957   4.165  0.00073 ***
Age            6.928      1.117   6.202 1.27e-05 ***
GenderM        7.204      3.251   2.216  0.04152 *  
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1 

Residual standard error: 7.061 on 16 degrees of freedom
Multiple R-squared: 0.7387,     Adjusted R-squared: 0.706 
F-statistic: 22.61 on 2 and 16 DF,  p-value: 2.176e-05
```

```
Call:
lm(formula = Height ~ Age + Gender1)

Residuals:
    Min      1Q  Median      3Q     Max 
-8.8462 -4.8523 -0.8102  3.3677 13.5058 

Coefficients:
            Estimate Std. Error t value Pr(>|t|)    
(Intercept)   69.495     15.135   4.592 0.000301 ***
Age            6.928      1.117   6.202 1.27e-05 ***
Gender1F      -7.204      3.251  -2.216 0.041517 *  
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1 

Residual standard error: 7.061 on 16 degrees of freedom
Multiple R-squared: 0.7387,     Adjusted R-squared: 0.706 
F-statistic: 22.61 on 2 and 16 DF,  p-value: 2.176e-05
```

The two models are exactly the same; only the way we look at the coefficient changes.

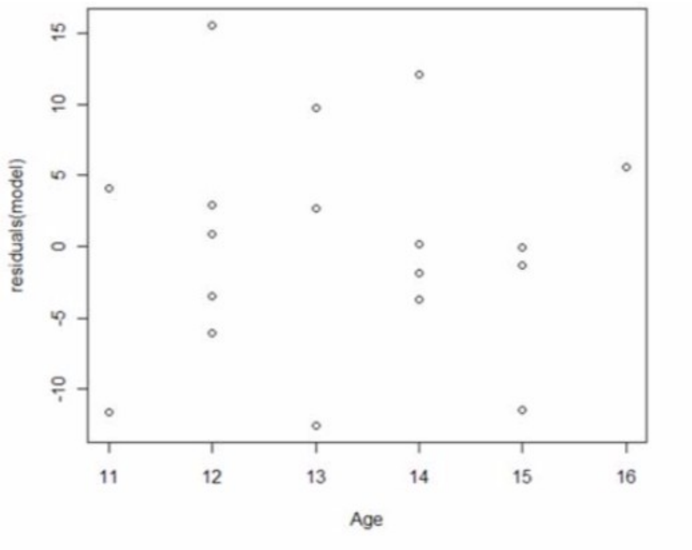
```
Gender1 <- relevel(Gender, ref="M")
```

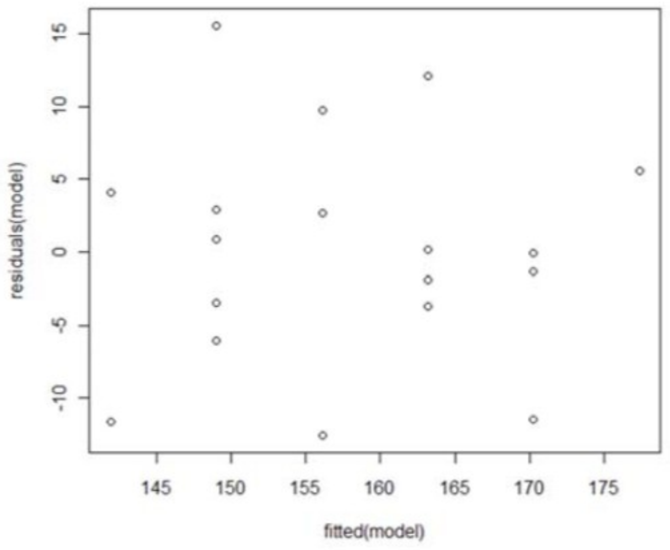
Diagnostic tools

It is always possible to fit a linear model and find a slope and intercept ... but it does not mean that the model is meaningful !

Examination of *residuals*: (which should show no obvious trend, since any systematic effect in the residuals should ideally be captured by the model):
– Normality
– Time effects
– Nonconstant variance – Curvature

Examination of *residuals*






```
plot( Age, residuals(model) )
```

```
plot( fitted(model), residuals(model) )
```

Works only for simple regression (only one variable on x axis)

Works also for multiple regression

High leverage ('influential') points are far from the center, and have potentially greater influence

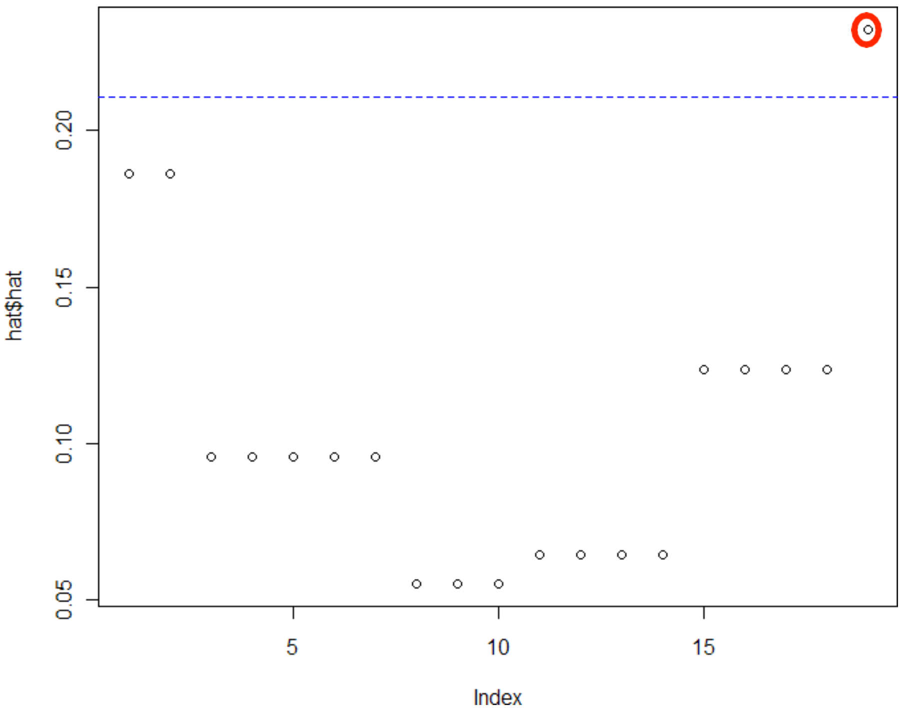
One way to assess points is through the *hat values* (obtained from the *hat matrix H*):

$$\hat{y} = Xb = X(X'X)^{-1}X'y = Hy$$

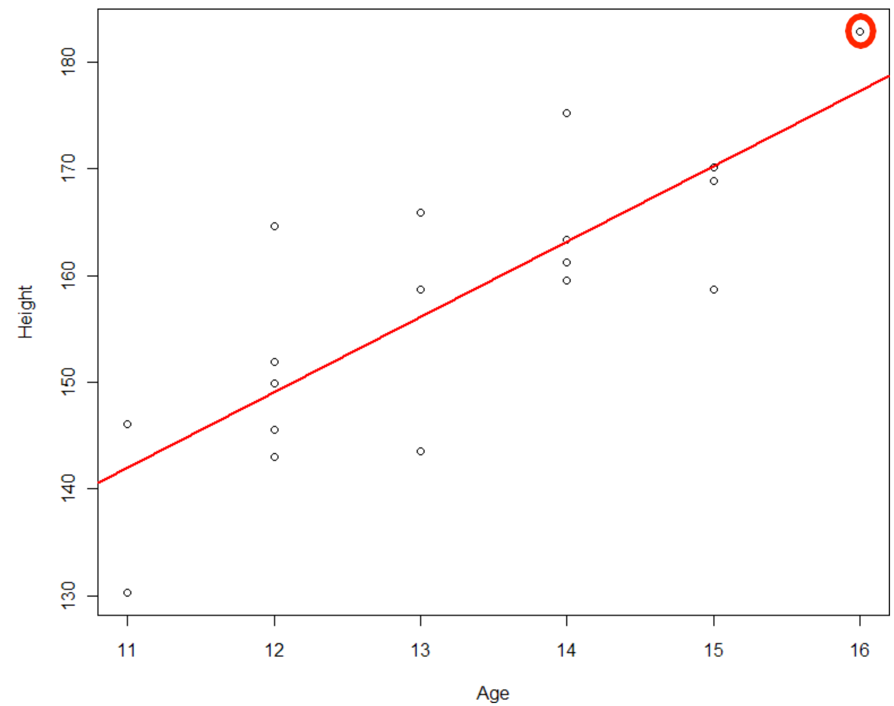
$$h_i = \Sigma_j h_{ij_2}$$

Average value of h = number of coefficients/n (including the intercept) = p/n

Cutoff typically 2p/n or 3p/n

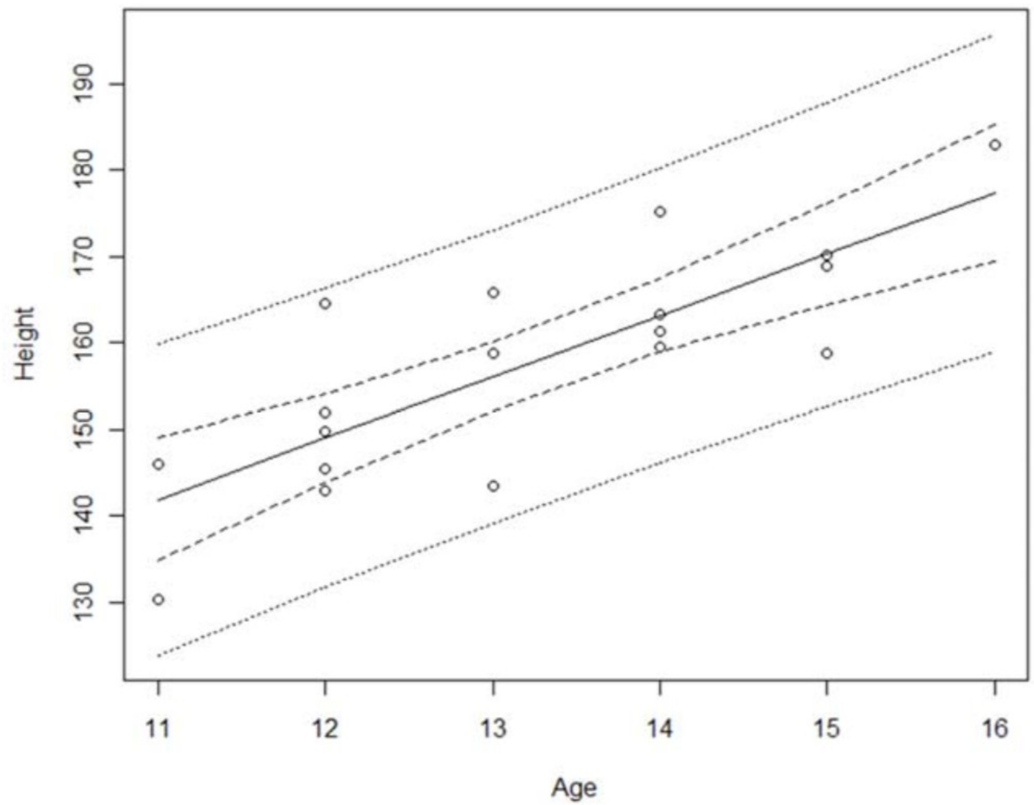


Hat values



Actual fit

```
>hat <- lm.influence( model )
>plot( hat$hat )
>abline(h=c(c(2,3)*2/19),lty=c(2,3),col=c("blue","red") )
```



Narrow bands: describe the uncertainly about the regression line

Wide bands: describe where most (95% by default) predictions would fall, assuming normality and constant variance.

In R: `?predict.lm`

If you want to learn more …

21
Apr
2021

Intermediate statistics: data analysis in practice

21 - 22 April 2021

Lausanne

UPCOMING