

Swiss Institute of Bioinformatics

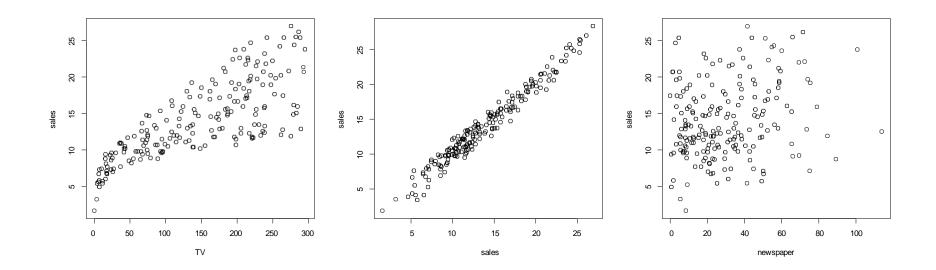
Introduction to statistics

Lausanne, January 2024

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Day 3: Correlation and Regression

Scatterplot



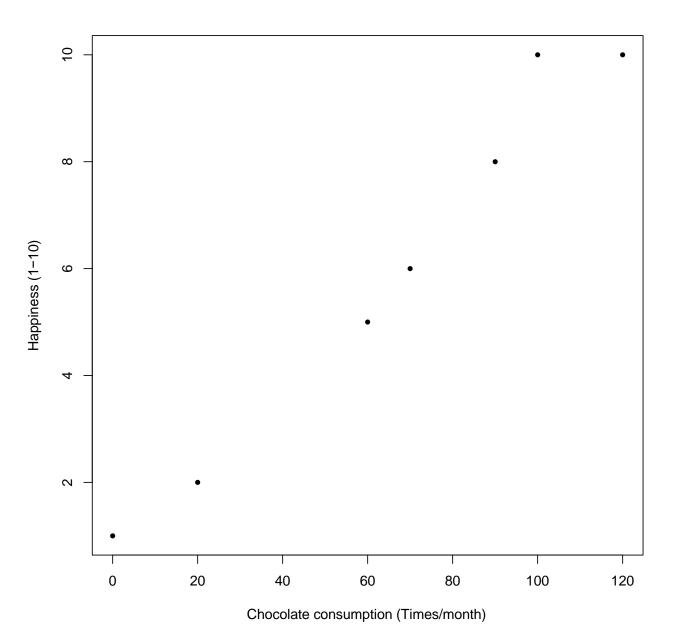
We are often interested in the statistical dependence between two variables, aka "correlation"

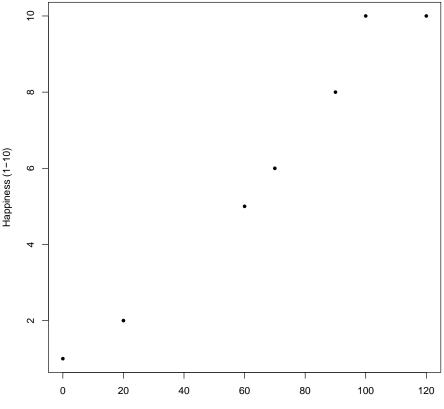
Pearson correlation

- 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 cov(X,Y)/sd(X)*sd(Y) which corresponds to a sort of 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)





Chocolate consumption (Times/month)

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

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

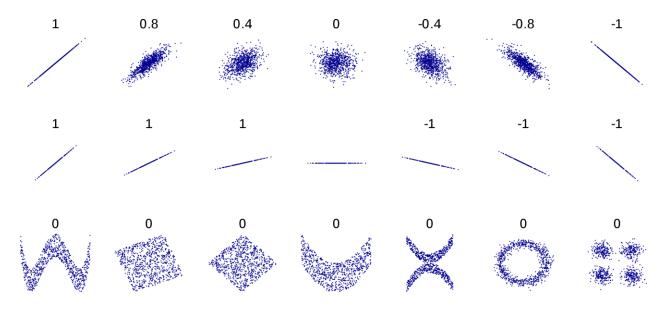


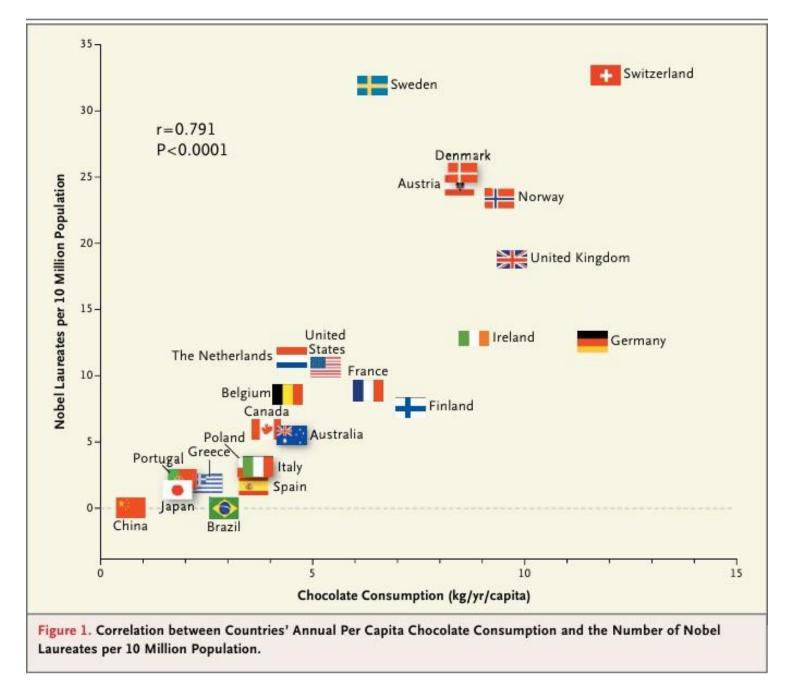
Image source: Wikipedia

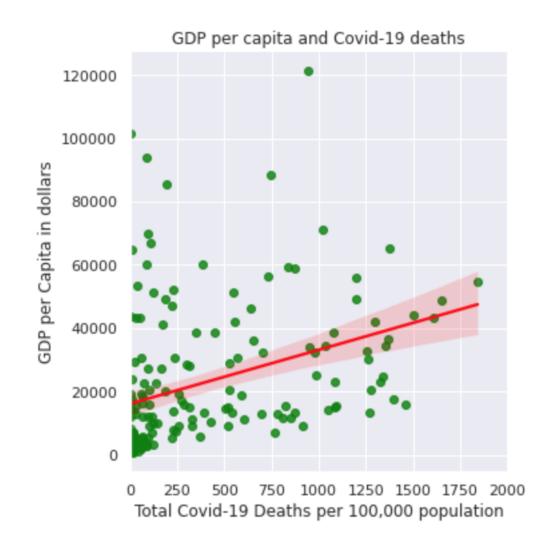
To recap ...

- *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)





https://towardsdatascience.com/coronavirus-correlations-5f49e5bb9710

CORRELATION IS NOT CAUSATION

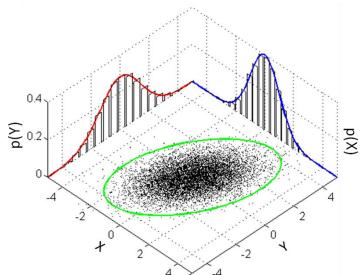
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Assumptions of Pearson correlation

• 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

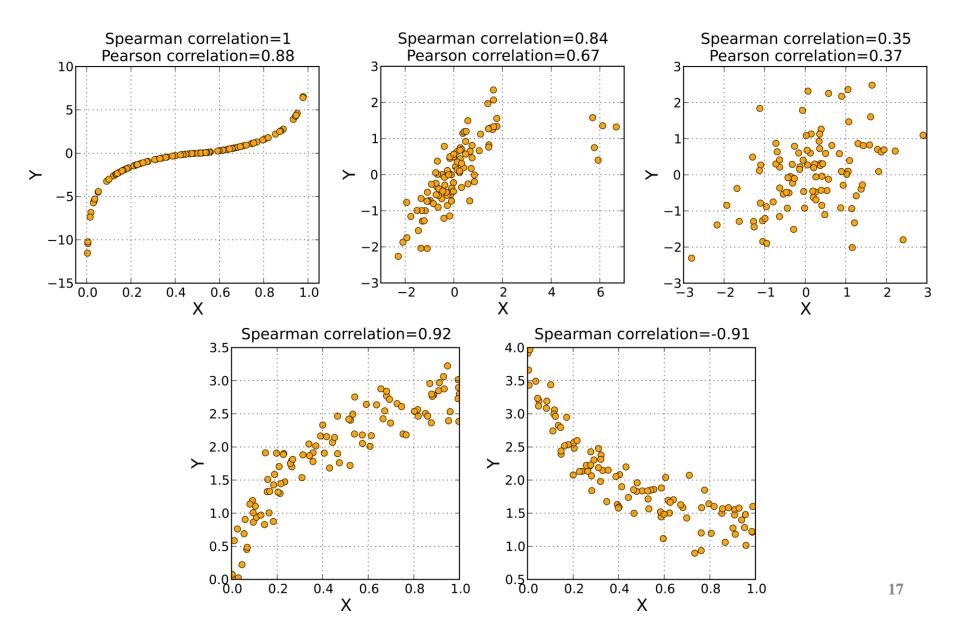
Spearman (rank) correlation

- A <u>nonparametric</u> measure of rank correlation
- The Spearman correlation coefficient (denoted by the Greek letter rho) is defined as the <u>Pearson correlation</u> <u>coefficient between the rank variables</u>

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</pre>
```

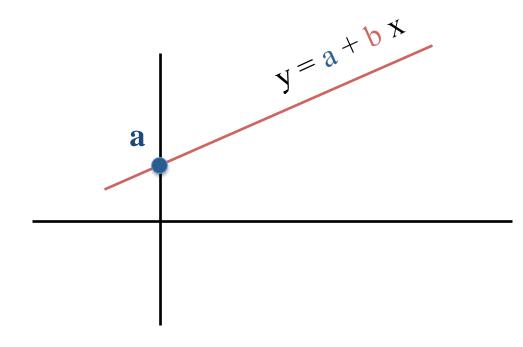
0.9085158

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

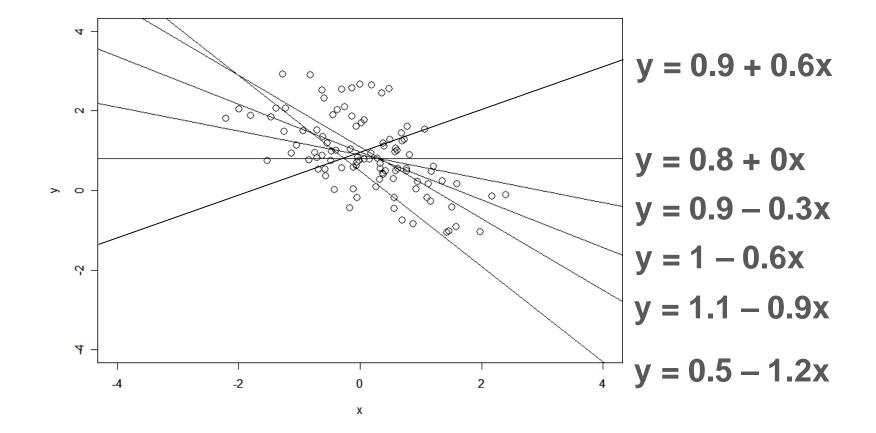
 Often it is useful to obtain a mathematical model that describes the association between variables, hence regression The equation for a line that can be used to predict y knowing x (in slope-intercept form) looks like

$$\mathbf{y} = \mathbf{a} + \mathbf{b} \mathbf{x}$$

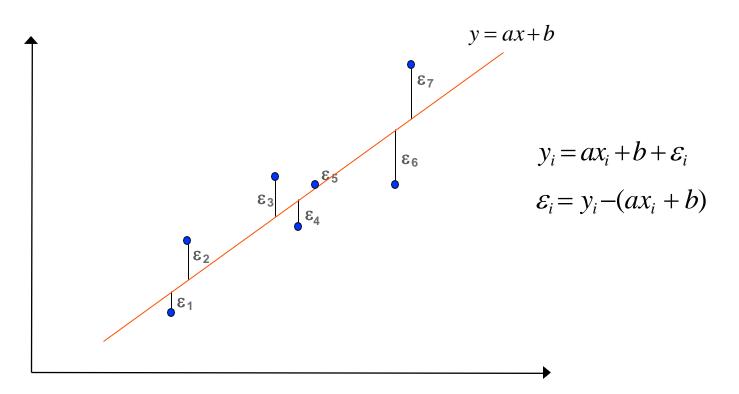
where *a* is called the *intercept* and *b* is the *slope*.



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



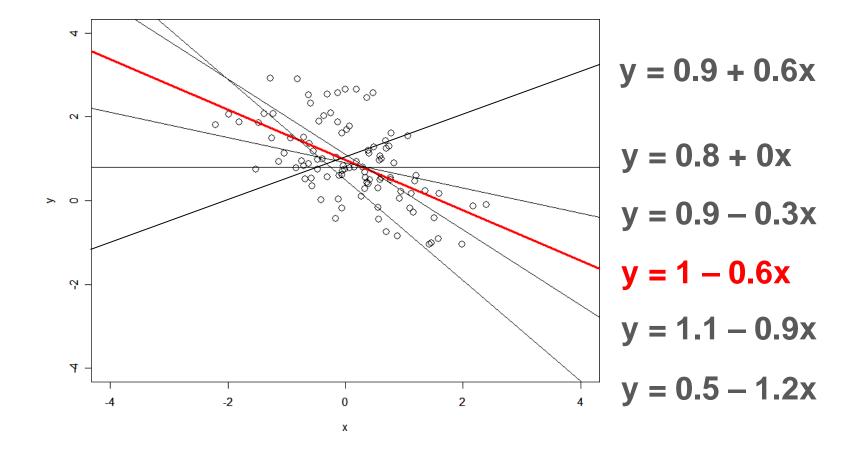
Least-squares approach to fit a line



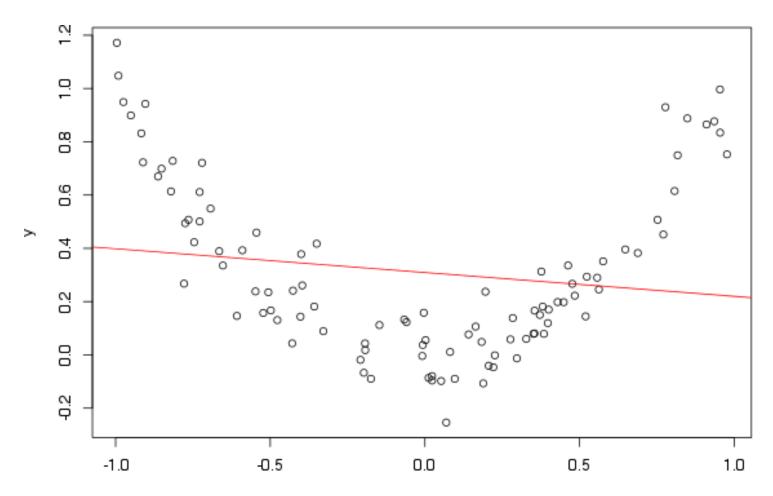
The least-squares procedure finds the straight line with the smallest sum of squares of vertical errors.

Finds a regression line such that $\sum_{i} \varepsilon_{i}^{2} = \varepsilon_{1}^{2} + \varepsilon_{2}^{2} + \varepsilon_{3}^{2} + \dots$ is minimum.

Over all possible straight lines, y= 1 - 0.6x is the "best" possible line according to least-squares criterion



What if the association is not linear?

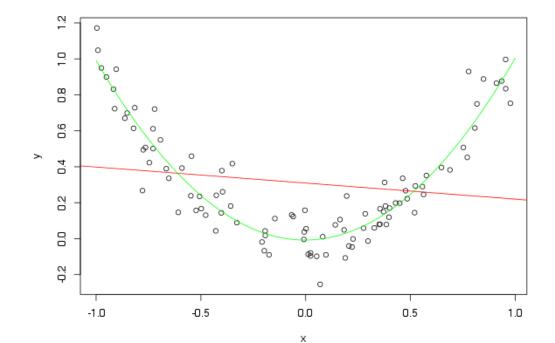


х

What if the data is not linear?

Use a polynomial regression

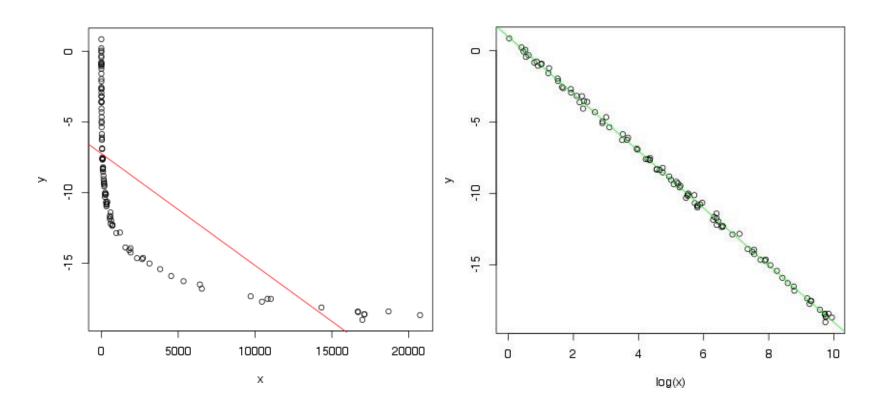
$$y = b_0 + b_1 x + b_2 x^2$$



What if the association is not linear?

Consider transforming the data (log)

log(y) = a + b x



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

 $+\mathcal{E}_i$

is equivalent to

$$\begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{bmatrix} = \begin{bmatrix} 1 & X_1 \\ 1 & X_2 \\ 1 & \vdots \\ 1 & X_n \end{bmatrix}$$

$$\left[\begin{array}{c}\beta_{0}\\\beta_{1}\\\vdots\\\vdots\\\varepsilon_{n}\end{array}\right]+\left[\begin{array}{c}\varepsilon_{1}\\\varepsilon_{2}\\\vdots\\\varepsilon_{n}\end{array}\right]$$

or $Y = X\beta + \epsilon$

$$Y_i = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} \cdot \qquad \qquad + \mathcal{E}_i$$

is equivalent to

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

or $Y = X\beta + \epsilon$

$$Y_{i} = \beta_{0} + \beta_{1}X_{i1} + \beta_{2}X_{i2} + \dots + \beta_{p-1}X_{ip-1} + \mathcal{E}_{i}$$

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 $Y = X\beta + \epsilon$

$$Y_{i} = \beta_{0} + \beta_{1}X_{i1} + \beta_{2}X_{i2} + \dots + \beta_{p-1}X_{ip-1} + \mathcal{E}_{i}$$

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

Least-square estimation of regression coefficients

Least-square estimation of regression coefficients

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

$$Y = X\beta + ε$$

X'Xβ = X'Y where $E{ε} = 0$

Least-square estimation of regression coefficients

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

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}$$
$$\mathbf{X'X}\boldsymbol{\beta} = \mathbf{X'Y} \quad \text{where} \quad E\{\boldsymbol{\varepsilon}\} = \mathbf{0}$$
$$\boldsymbol{\beta} = (\mathbf{X'X})^{-1}\mathbf{X'Y}$$

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 $\sim -1 + xvar1 + xvar2 + xvar3$

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

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

More on model formulas

Generic form

response ~ predictors

predictors can be numeric or categorical

R symbols to create formulas

- + to *add* morevariables
- 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

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

The CLASS dataset

> class

.

	Name	Gender	Age	Height	Weight
1	JOYCE	F	11	151.3	25.25
2	THOMAS	М	11	157.5	42.50
3	JAMES	М	12	157.3	41.50
4	JANE	F	12	159.8	42.25
5	JOHN	М	12	159.0	49.75
6	LOUISE	F	12	156.3	38.50
7	ROBERT	М	12	164.8	64.00
8	ALICE	F	13	156.5	42.00
9	BARBARA	F	13	165.3	49.00
10	JEFFREY	М	13	162.5	42.00
11	CAROL	F	14	162.8	51.25
12	HENRY	М	14	163.5	51.25
13	ALFRED	М	14	169.0	56.25
14	JUDY	F	14	164.3	45.00
15	JANET	F	15	162.5	56.25
16	MARY	F	15	166.5	56.00
17	RONALD	М	15	167.0	66.50
18	WILLIAM	М	15	166.5	56.00
19	PHILIP	М	16	172.0	75.00

The CLASS dataset

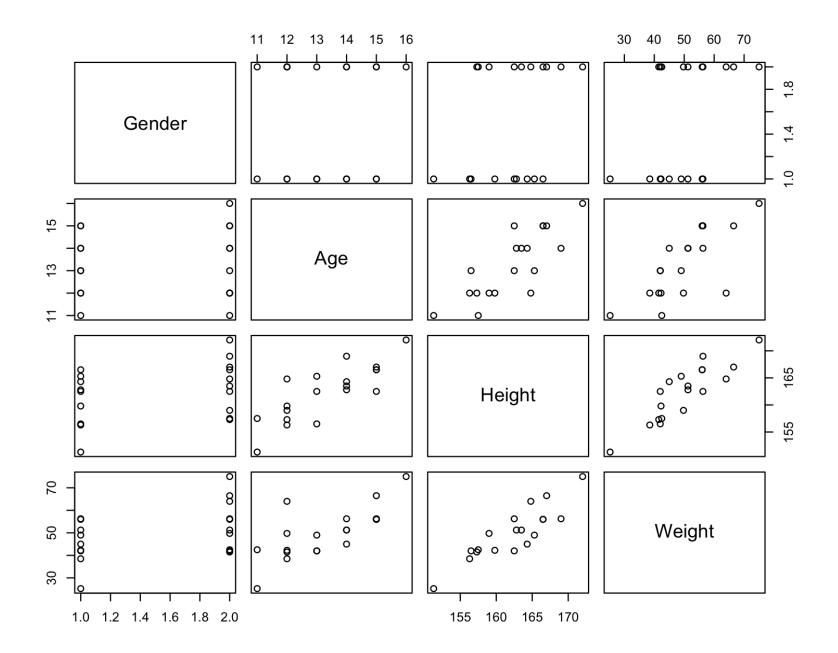
> summary(class)

Name		Gender		
Lengtł	n:19	Lengtł	n:19	
Class	:character	Class	:character	
Mode	:character	Mode	:character	

Ag	ge	He	Height			
Min.	:11.00	Min.	:151.3			
1st Qu	.:12.00	1st Qu	.:158.2			
Median	:13.00	Median	:162.8			
Mean	:13.32	Mean	:162.3			
3rd Qu	.:14.50	3rd Qu	.:165.9			
Max.	:16.00	Max.	:172.0			

Weight

Min. :25.25
1st Qu.:42.12
Median :49.75
Mean :50.01
3rd Qu.:56.12
Max. :75.00
> pairs(class[,-1])



Fitting the linear model in R

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

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

Coefficients: (Intercept) Age 125.224 2.787

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

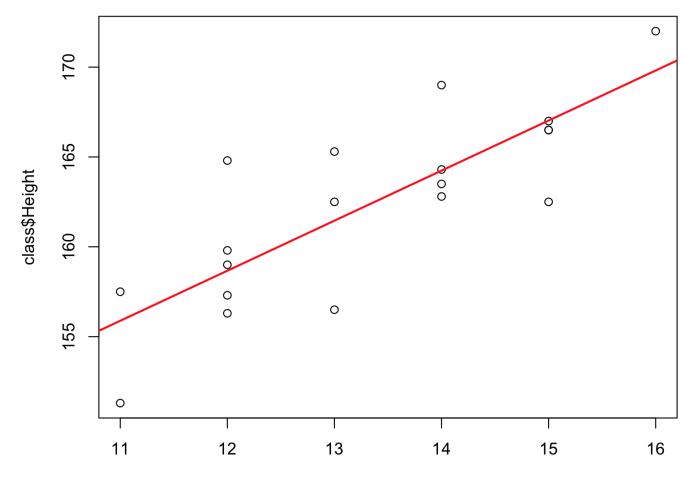
```
Call:
lm(formula = Height ~ Age, data = class)
```

Coefficients: (Intercept)

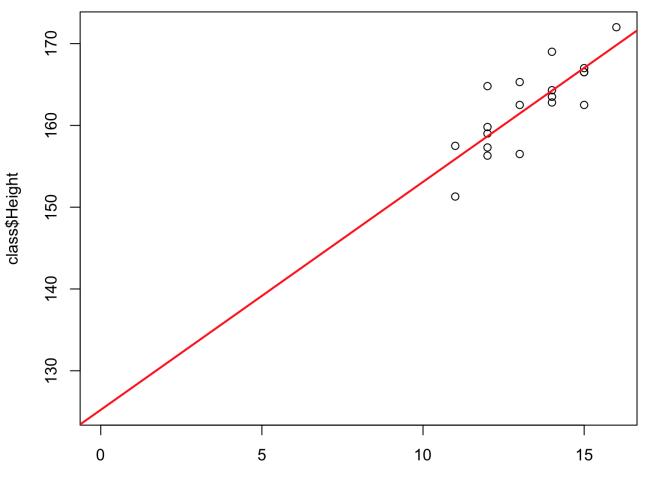
```
ercept) Age 125.224 2.787
```

Height = 125.224 + 2.787x 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 1m command in R

> summary(model)

Call: lm(formula = Height ~ Age, data = class)Residuals: Min 10 Median 30 Max -4.957 -1.407 -0.031 1.374 6.130 Coefficients: Estimate Std. Error t value Pr(>|t|) (Intercept) 125.2239 6.5217 19.201 5.82e-13 *** 2.7871 0.4869 5.724 2.48e-05 *** Age Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1 Residual standard error: 3.083 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

```
Function call
> summary(model)
Call:
lm(formula = Height ~ Age, data = class)
Residuals:
      1Q Median 3Q
  Min
                             Max
-4.957 -1.407 -0.031 1.374 6.130
Coefficients:
           Estimate Std. Error t value Pr(>|t|)
(Intercept) 125.2239 6.5217 19.201 5.82e-13 ***
            2.7871 0.4869 5.724 2.48e-05 ***
Age
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
Residual standard error: 3.083 on 17 degrees of freedom
```

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

Multiple R-squared: 0.6584, Adjusted R-squared: 0.6383

Example of summary results of the lm command in R

```
> summary(model)
```

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

```
Residuals:
Min 1Q Median 3Q Max
-4.957 -1.407 -0.031 1.374 6.130
```

Coefficients:

```
Estimate Std. Error t value Pr(>|t|)
(Intercept) 125.2239 6.5217 19.201 5.82e-13 ***
Age 2.7871 0.4869 5.724 2.48e-05 ***
---
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Residual standard error: 3.083 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

Distribution of the residuals

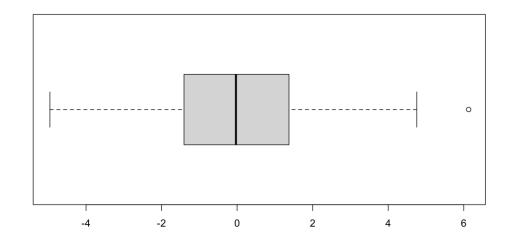
Five-number summary of the residuals equivalent to

> fivenum(residuals(model))

8 11 17 4 7 -4.95669291 -1.40669291 -0.03097113 1.37401575 6.13044619

or, graphically, using a boxplot:

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



Example of summary results of the 1m command in R

```
> summary(model)
```

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

Residuals: Min 1Q Median 3Q Max -4.957 -1.407 -0.031 1.374 6.130

Coefficients:						
	Estimate	Std. Error	t value	Pr(>ltl)		
(Intercept)	125.2239	6.5217	19.201	5.82e-13	***	
Age	2.7871	0.4869	5.724	2.48e-05	***	

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

Residual standard error: 3.083 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

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 1m command in R

```
> summary(model)
```

```
Call:
lm(formula = Height ~ Age, data = class)
Residuals:
  Min 10 Median 30
                             Max
-4.957 -1.407 -0.031 1.374 6.130
Coefficients:
           Estimate Std. Error t value Pr(>|t|)
(Intercept) 125.2239 6.5217 19.201 5.82e-13 ***
             2.7871 0.4869 5.724 2.48e-05 ***
Age
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
Residual standard error: 3.083 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 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

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] 2.996486

sqrt(sum(residuals(model)^2)/18)

[1] 2.996486

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

- > sqrt(sum(residuals(model)^2)/17)
- [1] 3.083359

Example of summary results of the 1m command in R

```
> summary(model)
```

```
Call:
lm(formula = Height ~ Age, data = class)
Residuals:
  Min 10 Median 30
                             Max
-4.957 -1.407 -0.031 1.374 6.130
Coefficients:
           Estimate Std. Error t value Pr(>|t|)
(Intercept) 125.2239 6.5217 19.201 5.82e-13 ***
             2.7871 0.4869 5.724 2.48e-05 ***
Age
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
Residual standard error: 3.083 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
```

R² is the proportion of the total variance in the response data that is explained by the model

if R²=1, the data fits perfectly on a straight line, and the model explains all the variance

 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

In the case of simple regression, it is equal to the square of the correlation coefficient between the two variables:

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

R² is the proportion of the total variance in the response data that is explained by the model

if R²=1, the data fits perfectly on a straight line, and the model explains all the variance

In the case of simple regression, it is equal to the square of the correlation coefficient between the two variables:

> summary(model)\$r.squared
[1] 0.6584257
> cor(class\$Age,class\$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 1m command in R

```
> summary(model)
```

```
Call:
lm(formula = Height ~ Age, data = class)
Residuals:
  Min 10 Median 30
                             Max
-4.957 -1.407 -0.031 1.374 6.130
Coefficients:
           Estimate Std. Error t value Pr(>|t|)
(Intercept) 125.2239 6.5217 19.201 5.82e-13 ***
             2.7871 0.4869 5.724 2.48e-05 ***
Age
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
Residual standard error: 3.083 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
```

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.

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.



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, data = class)Residuals: Min 10 Median 30 Max -3.6248 -1.3016 -0.0176 0.8324 4.1019 Coefficients: Estimate Std. Error t value Pr(>|t|) (Intercept) 132.1943 5.0823 26.011 1.61e-14 *** 1.2267 0.5302 2.314 0.03431 * Age Weight 0.2761 0.0695 3.973 0.00109 ** Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 2.255 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 <u>separately</u>.

Coefficients: Estimate Std. Error t value Pr(>|t|) (Intercept) 132.1943 5.0823 26.011 1.61e-14 *** Age 1.2267 0.5302 2.314 0.03431 * Weight 0.2761 0.0695 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 S	Std. Error t	value Pr(>ltl)	
(Intercept)	142.57014	2.67989 5	53.200 <	2e-16 ***	
Weight	0.39523	0.05231	7.555 7.8	9e-07 ***	
Coefficient	s:				
	Estimate	Std. Error t	t value P	r(> t)	
(Intercept)		6.5217			**
Age	2.7871	0.4869	5.724 2	.48e-05 *	**
Coefficient	s:				
	Estimate	Std. Error	t value	Pr(>ltl)	
(Intercept)	132.1943	5.0823	26.011	1.61e-14	***
Age	1.2267	0.5302	2.314	0.03431	*
Weight	0.2761	0.0695	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. 61

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

As before, R² 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 R², up to 1 when there the number of degrees of freedom is 0 (number of parameters to estimate = number of observations).

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.

 $R^2 = 1 - \frac{SS_{residuals}}{SS_{total}}$

It is always equal or below R².

Adjusted R² = 1 -
$$\frac{SS_{residuals}(n-K)}{SS_{total}(n-1)}$$

Example

y <- rnorm(10) x1 <- rnorm(10); x2 <- rnorm(10); ...; x9 <rnorm(10)</pre>

summary(lm(y ~ x1)); summary(lm(y ~ x1+x2));

1:	Multiple	R-squared:	0.1419,
2:	Multiple	R-squared:	0.5173,
3:	Multiple	R-squared:	0.557,
4:	Multiple	R-squared:	0.5577,
5:	Multiple	R-squared:	0.7953,
6:	Multiple	R-squared:	0.8321,
7:	Multiple	R-squared:	0.984,
8:	Multiple	R-squared:	0.9851,
9:	Multiple	R-squared:	1,

Adjusted	R-squared:	0.03464
Adjusted	R-squared:	0.3794
Adjusted	R-squared:	0.3355
Adjusted	R-squared:	0.2039
Adjusted	R-squared:	0.5395
Adjusted	R-squared:	0.4962
Adjusted	R-squared:	0.9281
Adjusted	R-squared:	0.866
Adjusted	R-squared:	NaN

The last regression from the example

Call: lm(formula = $y \sim x1 + x2 + x3 + x4 + x5 + x6 + x7 + x8 + x9)$					
Residuals:	1				,
	duals are 0: no	residual	degrees	of freedo	m !
Coofficient	- •				
Coefficient		<u> </u>			
	Estimate Std.	Error t v	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	
x 6	-0.65387	NA	NA	NA	
x7	-0.48271	NA	NA	NA	
x8	-0.62487	NA	NA	NA	
x9	0.23759	NA	NA	NA	
				freedom	
	andard error: N		-		
Multiple R-	squared: 1,	Adj	usted R-s	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 or	2 and 16 DF,	p-va	alue: 7.64	6e-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 Ftest 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

Categorical variables

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

$Height = b_0 + b_1 Age + b_2 \ll Gender \gg + error$

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

Categorical variables

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

Height = $b_0 + b_1 Age + b_2 \ll Gender \gg + error$

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

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

Example of summary results of the 1m command in R

Call: lm(formula = Height ~ Age + Gender, data = class)Residuals: 10 Median 30 Min Max -3.483 -1.910 -0.319 1.326 5.317 Coefficients: Estimate Std. Error t value Pr(>|t|) (Intercept) 124.5241 5.8886 21.147 4.04e-13 *** Age 2.7276 0.4398 6.202 1.27e-05 *** GenderM 2.8362 1.2797 2.216 0.0415 * Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1 Residual standard error: 2.78 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

Example of summary results of the lm command in R

Call: lm(formula = Height ~ Age + Gender, data = class)Residuals: Min 10 Median 30 Max baseline for -3.483 -1.910 -0.319 1.326 5.317 height among Female Coefficients: Estimate Std. Error t value Pr(>|t|) 5.8886 21.147 4.04e-13 *** (Intercept) 124.5241 2.7276 0.4398 6.202 1.27e-05 *** Age GenderM 2.8362 1.2797 2.216 0.0415 * 0 (**** 0.001 (*** 0.01 (** 0.05 (. 0.1 (1 Signif. codes:

Residual standard error: 2.78 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 Example of summary results of the lm command in R

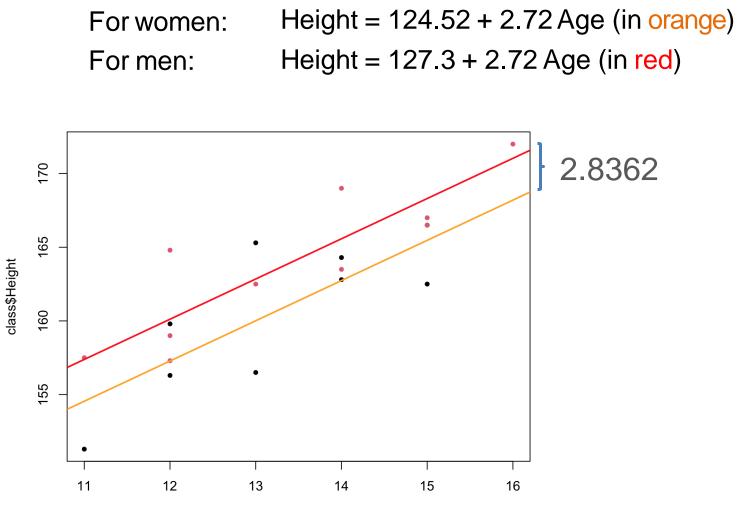
Call: lm(formula = Height ~ Age + Gender, data = class)						
Residuals: Min 1Q -3.483 -1.910	Median -0.319 1.	•				baseline for height among
Coefficients:						Female
	stimate Std					
(Intercept) 12	24.5241	5.8886	21.147	4.04e-13	*** 🖌	
Age	2.7276			1.27e-05		_
GenderM	2.8362	1.2797	2.216	0.0415	*]
 Sianif. codes	: 0 '***'	0.001 '**	*' 0.01	·*' 0.05	·.' 0	.1 ' ' 1

Residual standard error: 2.78 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 factor GenderM corresponds to the difference in baseline for Males compared to females

Graphical interpretation

The model specifies 2 straight lines, with the same slope but different yintercepts:



class\$Age

What if we don't use a linear model?

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

This result is slightly different from the 2.8362 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.

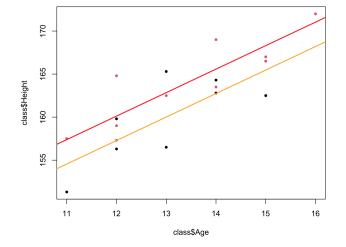
If this assumption is incorrect, it means that there is an *interaction* between the factors « age » and « gender », that is, the effect of age is different depending on the gender.

Interactions are modeled in R in the following way:

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

which is equivalent to

Im(formula = Height ~ Age * Gender)



Coefficients with an interaction

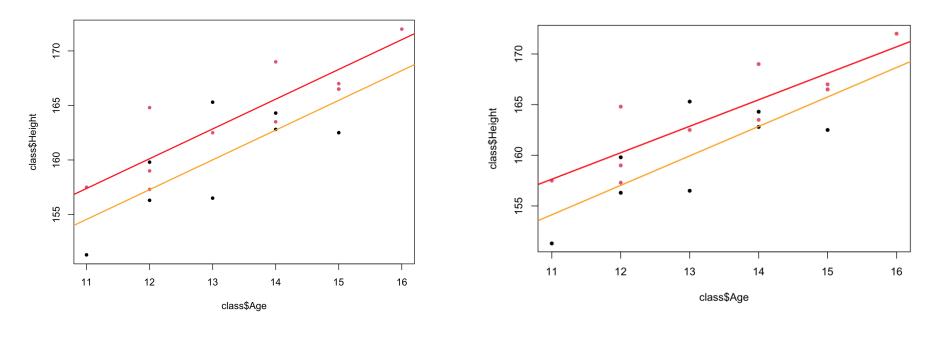
Call: lm(formula = Height ~ Age * Gender, data = class) Residuals: 10 Median 30 Min Max -3.4429 -1.7844 -0.3648 1.3730 5.3571 Coefficients: Estimate Std. Error t value Pr(>|t|) (Intercept) 122.1500 9.6409 12.670 2.05e-09 *** 2.9071 0.7256 4.007 0.00114 ** Age GenderM 6.7443 12.4109 0.543 0.59483 Age:GenderM -0.2940 0.9285 -0.317 0.75585 _ _ _ Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1 Residual standard error: 2.862 on 15 degrees of freedom Multiple R-squared: 0.7404, Adjusted R-squared: 0.6885 F-statistic: 14.26 on 3 and 15 DF, p-value: 0.0001152

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

> model <- lm(Height ~ Age+Gender1, data=class)</pre> > summary(model) Call: lm(formula = Height ~ Age + Gender1, data = class) Residuals: Min 10 Median 30 Max -3.483 -1.910 -0.319 1.326 5.317 Coefficients: Estimate Std. Error t value Pr(>|t|) (Intercept) 127.3603 5.9587 21.374 3.43e-13 *** 2.7276 0.4398 6.202 1.27e-05 *** Age Gender1F -2.8362 1.2797 -2.216 0.0415 * _ _ _ Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1 Residual standard error: 2.78 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 > model <- lm(Height ~ Age+Gender, data=class)</pre> > summary(model) Call: lm(formula = Height ~ Age + Gender, data = class)Residuals: Min 1Q Median 30 Max -3.483 -1.910 -0.319 1.326 5.317 Coefficients: Estimate Std. Error t value Pr(>|t|) (Intercept) 124.5241 5.8886 21.147 4.04e-13 *** 2.7276 0.4398 6.202 1.27e-05 *** Age GenderM 2.8362 1.2797 2.216 0.0415 * ___ Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1 Residual standard error: 2.78 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")

What if Males were the baseline ?

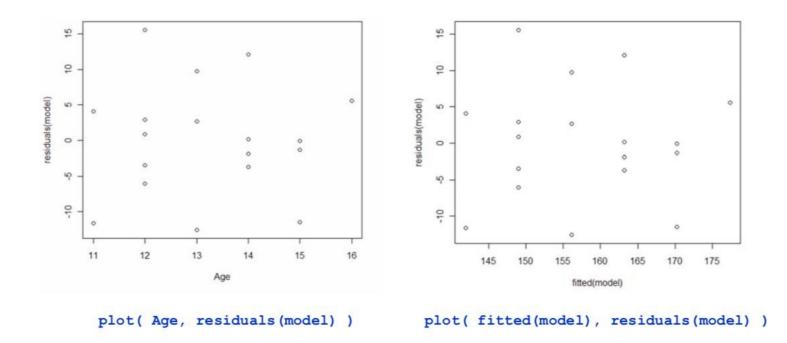
Diagnostic tools

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*



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

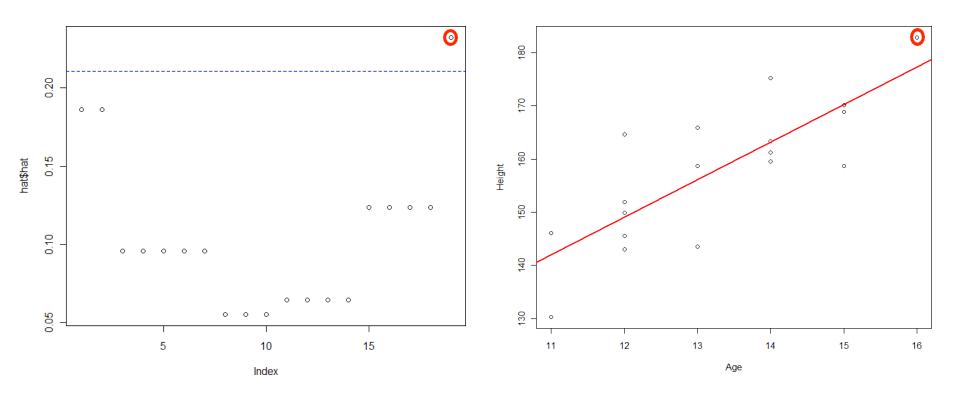
One way to assess points is through the *hat values* (obtained from the *hat matrix H*):

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

 $h_i = \Sigma_j h_{ij_2}$

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

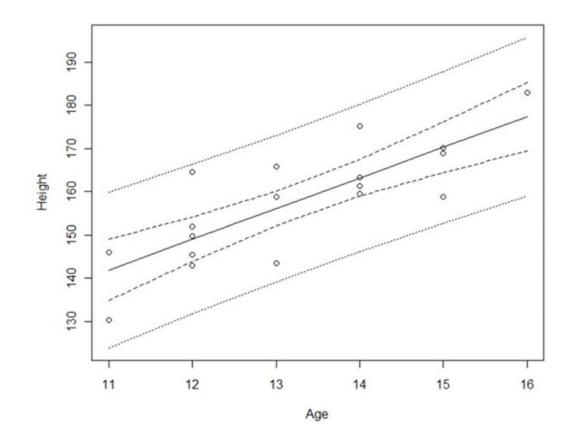
Cutoff typically 2p/n or 3p/n



Hat values

Actual fit

>hat <- Im.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 lineWide bands:describe where most (95% by default) predictions would fall,
assuming normality and constant variance.

In R: ?predict.lm