

# Multivariate Statistics in Ecology and Quantitative Genetics

## **3. Linear Regression and Linear Models**

Dirk Metzler & Martin Hutzenthaler

<http://evol.bio.lmu.de/StatGen.html>

19. Mai 2010

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## Regression toward the mean

Univariate linear regression: how and why?

t-test for linear regression

Examples with transformed variables

- log-scaling brain sizes and body weights

- root of numbers of inhabitants and deaths

Multivariate Regression

- Example: species richness on sandy beaches

- Example: Success of different therapies

- Example: Daphnia

Cross validation and AIC

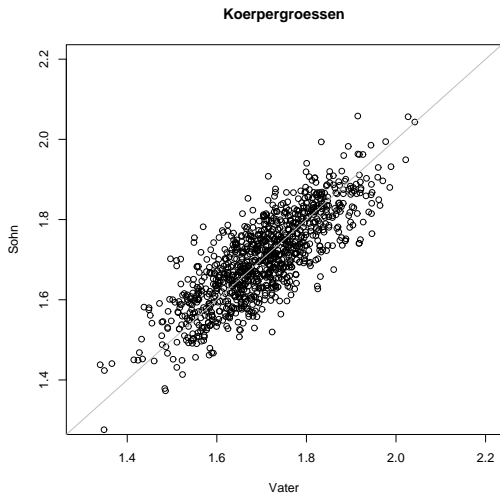
# Origin of the word “Regression”

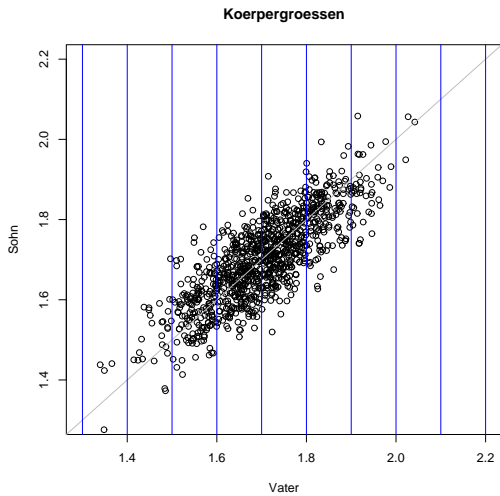
Sir Francis Galton (1822–1911): Regression toward the mean.

# Origin of the word “Regression”

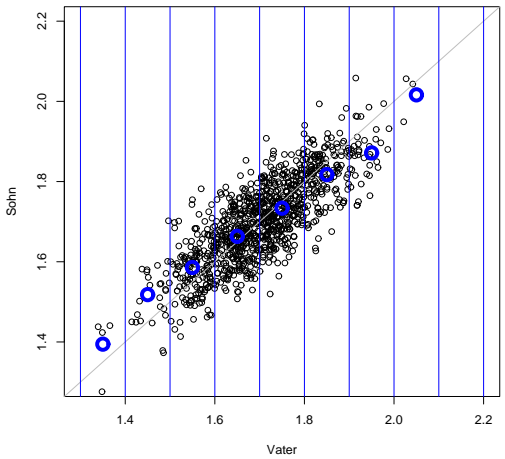
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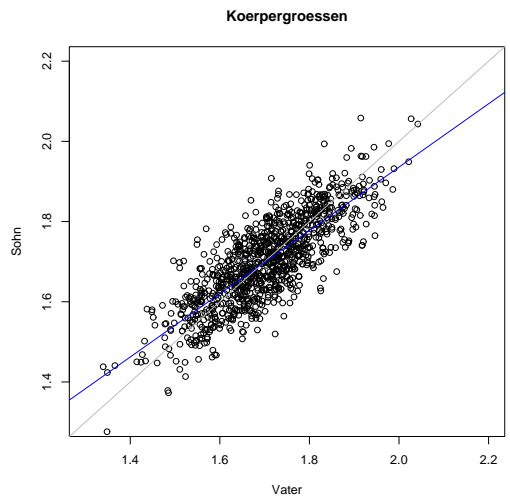
Tall fathers tend to have sons that are slightly smaller than the fathers. Sons of small fathers are on average larger than their fathers.



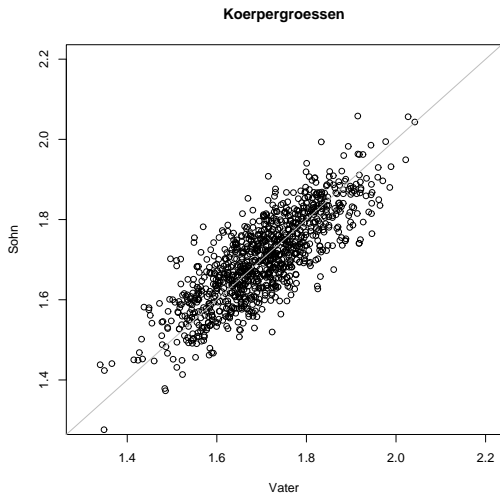


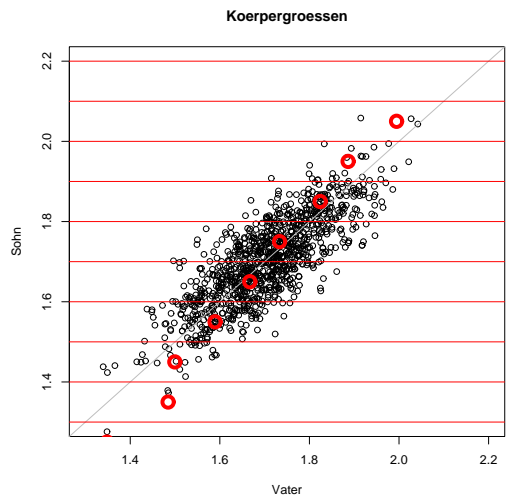
### Koerpergroessen

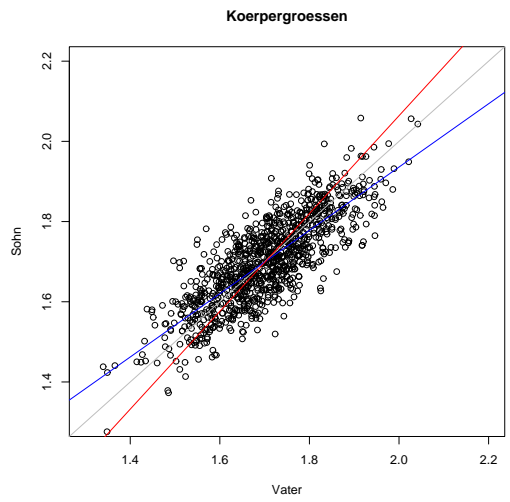


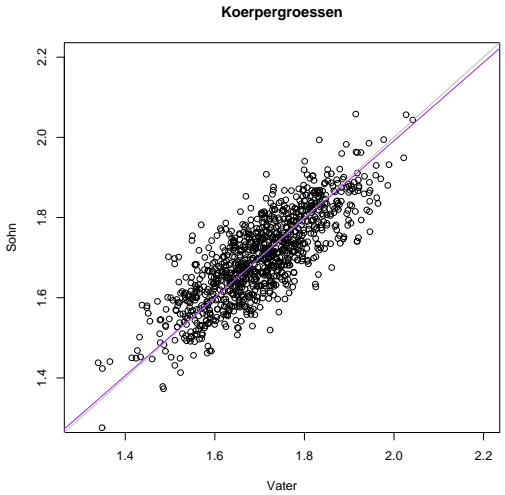












## Similar effects

- ▶ In sports: The champion of the season will tend to fail the high expectations in the next year.

# Similar effects

- ▶ In sports: The champion of the season will tend to fail the high expectations in the next year.
- ▶ In school: If the worst 10% of the students get extra lessons and are not the worst 10% in the next year, then this does not proof that the extra lessons are useful.

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Cross validation and AIC



photo (c) by Jörg Hempel

Griffon Vulture  
*Gypus fulvus*  
German:  
Gänsegeier





Prinzinger, R., E. Karl, R. Bögel, Ch. Walzer (1999): Energy metabolism, body temperature, and cardiac work in the Griffon vulture *Gyps vulvus* - telemetric investigations in the laboratory and in the field.

*Zoology* **102**, Suppl. II: 15

- ▶ Data from Goethe-University, Group of Prof. Prinzinger
- ▶ Developed telemetric system for measuring heart beats of flying birds



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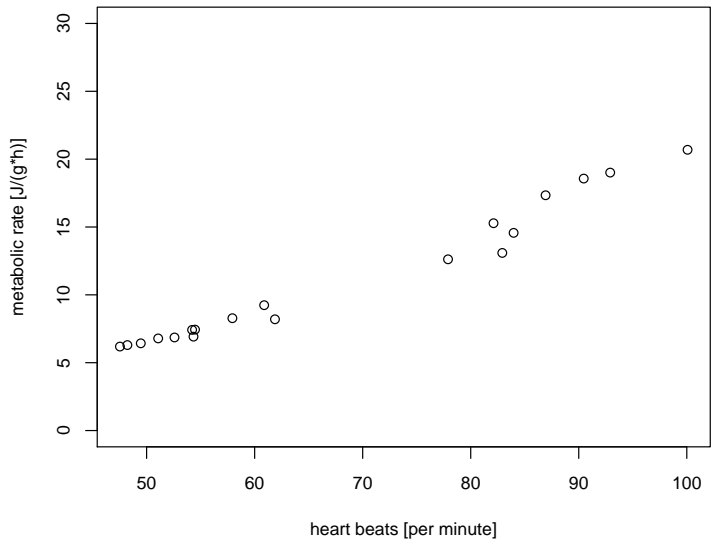


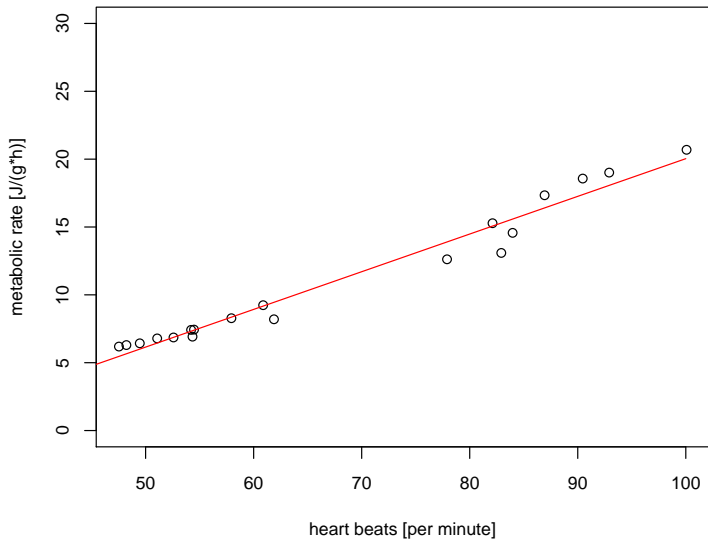
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- ▶ Developed telemetric system for measuring heart beats of flying birds
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- ▶ metabolic rate can only be measured in the lab
- ▶ can we infer metabolic rate from heart beat frequency?

### griffon vulture, 17.05.99, 16 degrees C



**griffon vulture, 17.05.99, 16 degrees C**

vulture

	day	heartbpm	metabol	minTemp	maxTemp	medtemp
1	01.04./02.04.	70.28	11.51	-6	2	-2.0
2	01.04./02.04.	66.13	11.07	-6	2	-2.0
3	01.04./02.04.	58.32	10.56	-6	2	-2.0
4	01.04./02.04.	58.63	10.62	-6	2	-2.0
5	01.04./02.04.	58.05	9.52	-6	2	-2.0
6	01.04./02.04.	66.37	7.19	-6	2	-2.0
7	01.04./02.04.	62.43	8.78	-6	2	-2.0
8	01.04./02.04.	65.83	8.24	-6	2	-2.0
9	01.04./02.04.	47.90	7.47	-6	2	-2.0
10	01.04./02.04.	51.29	7.83	-6	2	-2.0
11	01.04./02.04.	57.20	9.18	-6	2	-2.0
.	.	.	.	.	.	.
.	.	.	.	.	.	.
.	.	.	.	.	.	.

(14 different days)

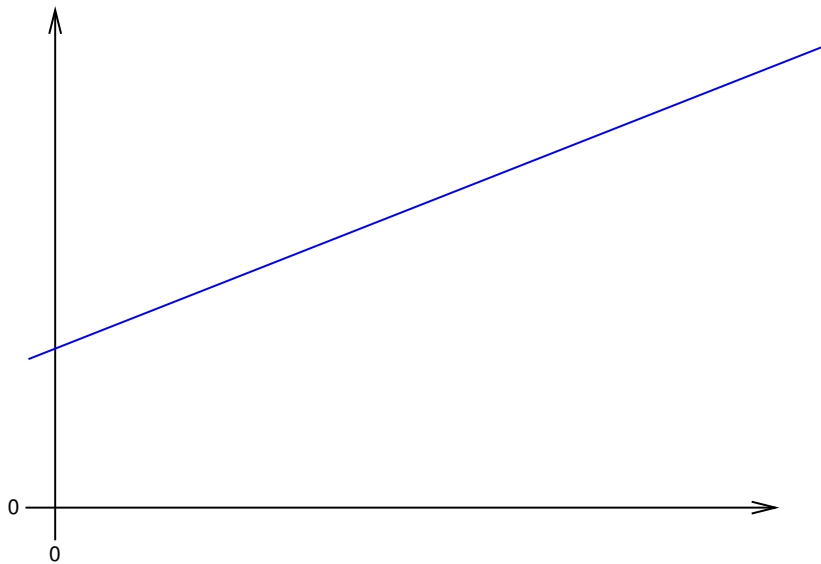
```

> model <- lm(metabol~heartbpm,data=vulture,
              subset=day=="17.05.")
> summary(model)
Call:
lm(formula = metabol ~ heartbpm, data = vulture, subset = day
    "17.05.")
Residuals:
    Min       1Q   Median       3Q      Max
-2.2026 -0.2555  0.1005  0.6393  1.1834
Coefficients:
              Estimate Std. Error t value Pr(>|t|)
(Intercept) -7.73522     0.84543  -9.149 5.60e-08 ***
heartbpm     0.27771     0.01207  23.016 2.98e-14 ***
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1 1
Residual standard error: 0.912 on 17 degrees of freedom
Multiple R-squared:  0.9689, Adjusted R-squared:  0.9671
F-statistic: 529.7 on 1 and 17 DF,  p-value: 2.979e-14

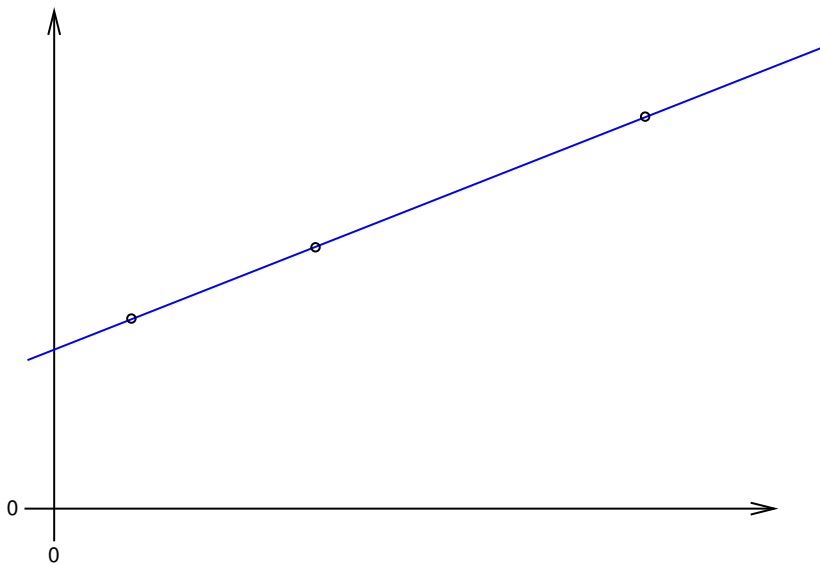
```



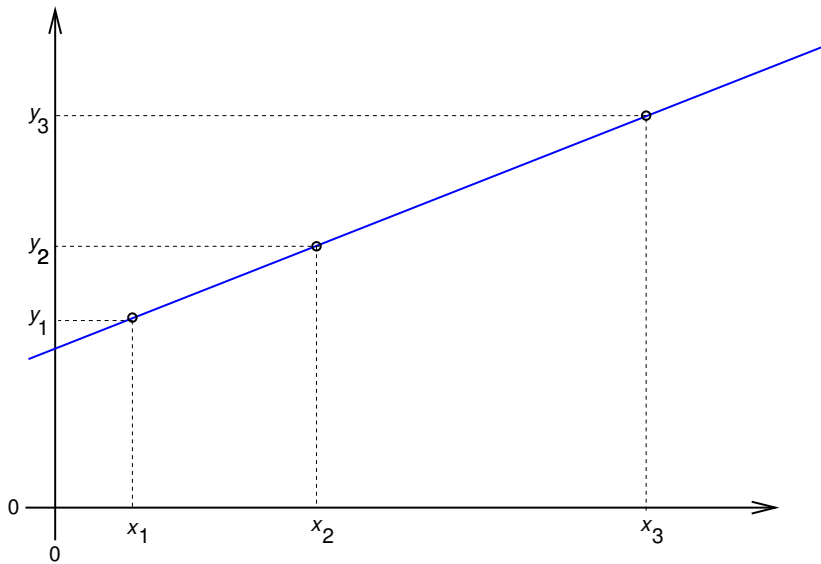
# Univariate linear regression: how and why?



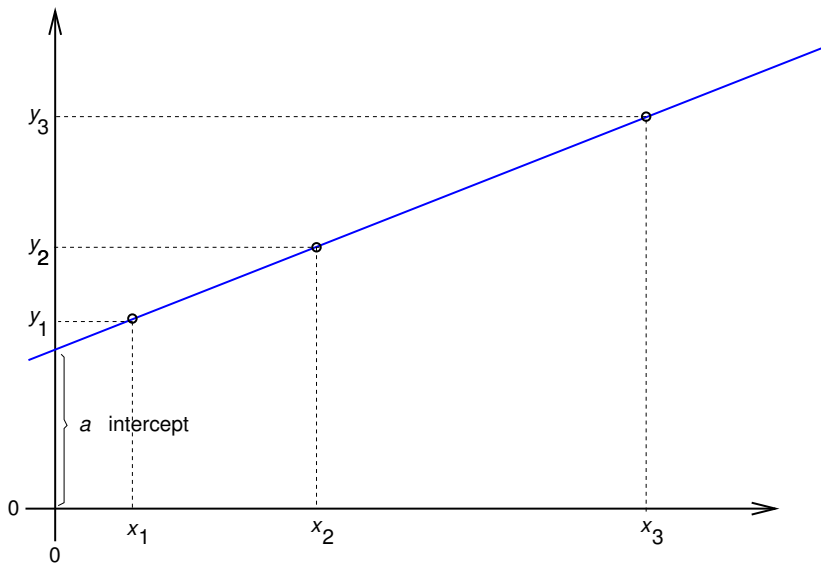
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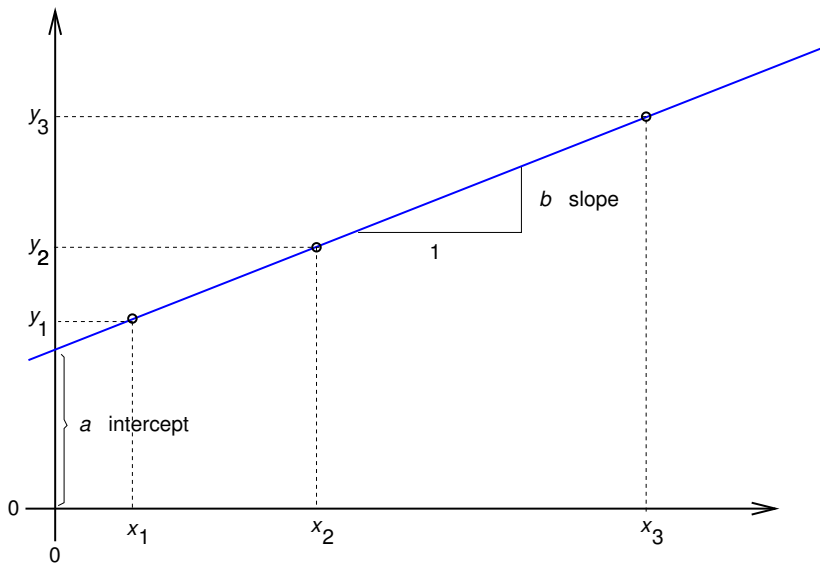
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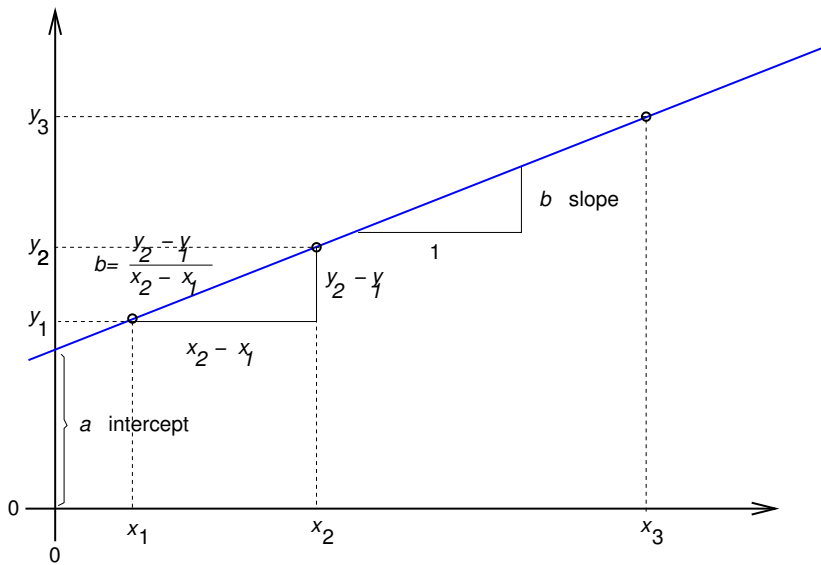
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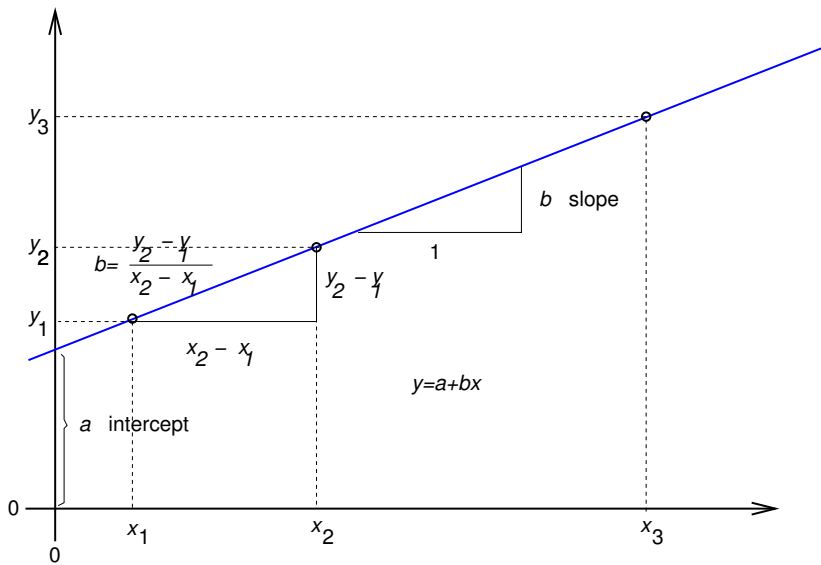
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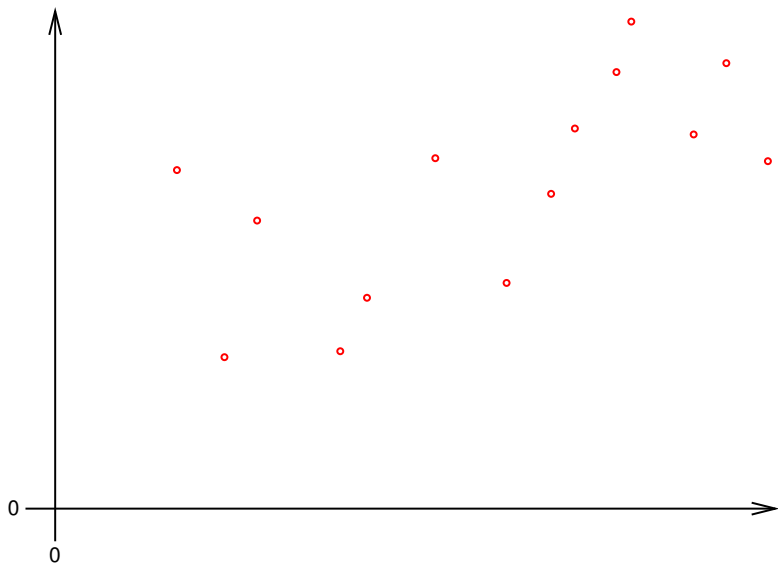
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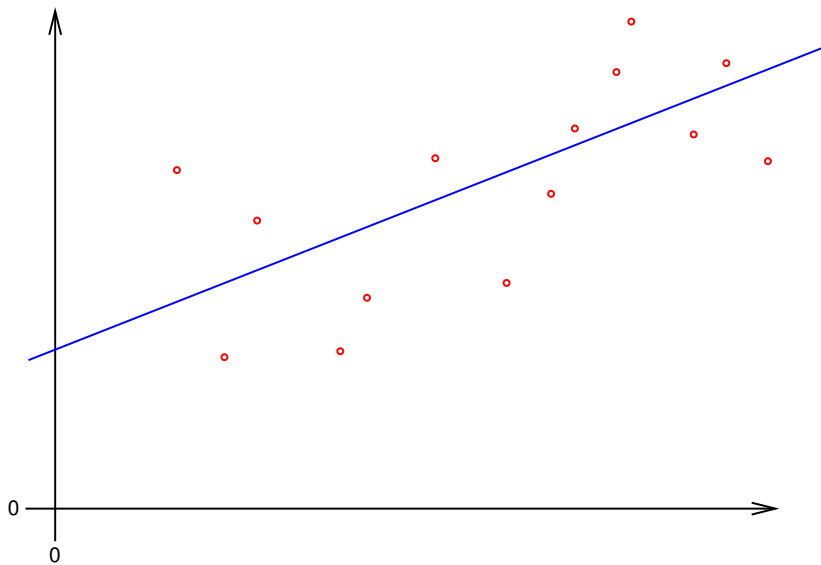


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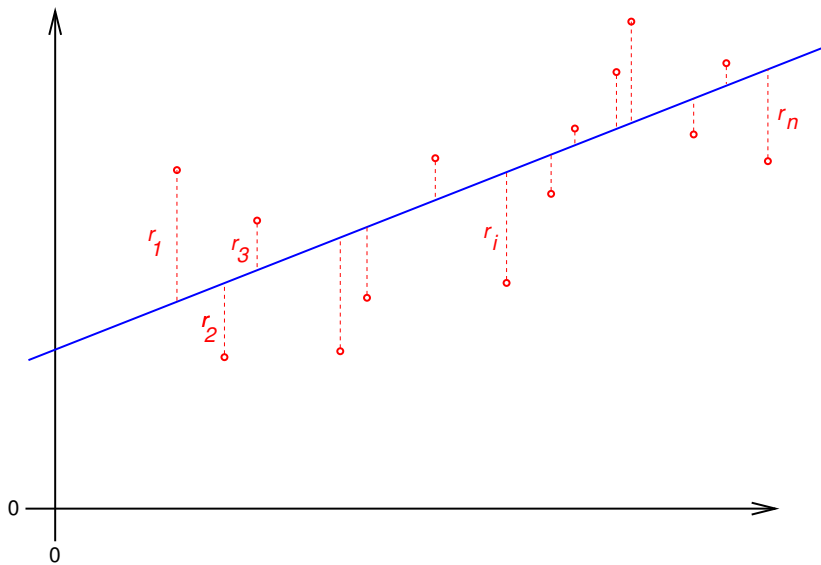




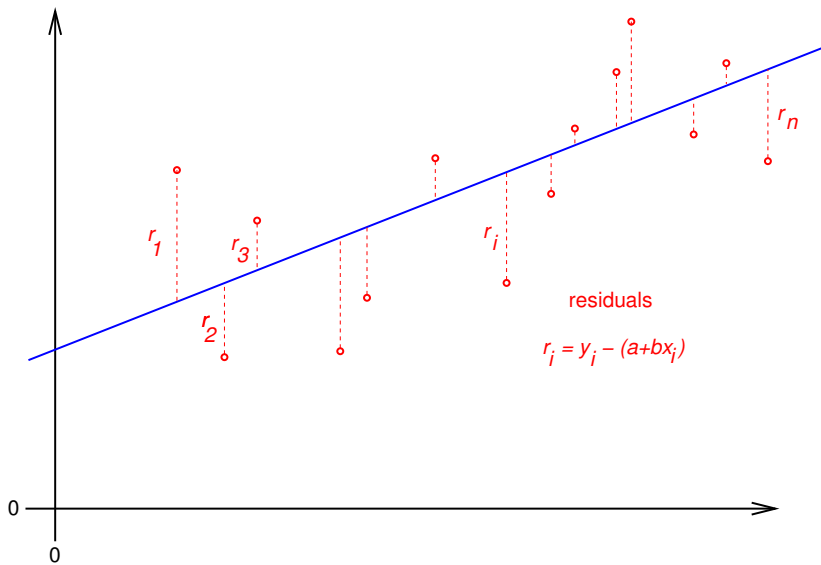
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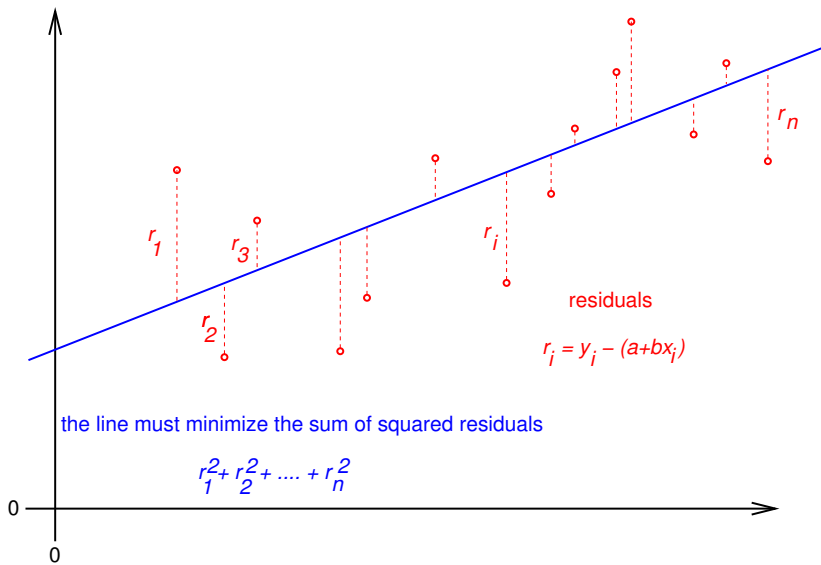


# Univariate linear regression: how and why?



# Univariate linear regression: how and why?





define the regression line

$$y = \hat{a} + \hat{b} \cdot x$$

by minimizing the sum of squared residuals:

$$(\hat{a}, \hat{b}) = \arg \min_{(a,b)} \sum_i (y_i - (a + b \cdot x_i))^2$$

this is based on the model assumption that values  $a, b$  exist, such that, for all data points  $(x_i, y_i)$  we have

$$y_i = a + b \cdot x_i + \varepsilon_i,$$

whereas all  $\varepsilon_i$  are independent and normally distributed with the same variance  $\sigma^2$ .

given data:

<b>Y</b>	<b>X</b>
$y_1$	$x_1$
$y_2$	$x_2$
$y_3$	$x_3$
$\vdots$	$\vdots$
$y_n$	$x_n$

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Model: there are values  
 $a, b, \sigma^2$  such that

$$y_1 = a + b \cdot x_1 + \varepsilon_1$$

$$y_2 = a + b \cdot x_2 + \varepsilon_2$$

$$y_3 = a + b \cdot x_3 + \varepsilon_3$$

$$\vdots \quad \quad \quad \vdots$$

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$\varepsilon_1, \varepsilon_2, \dots, \varepsilon_n$  are independent  $\sim \mathcal{N}(0, \sigma^2)$ .



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$\Rightarrow y_1, y_2, \dots, y_n$  are independent  $y_i \sim \mathcal{N}(a + b \cdot x_i, \sigma^2)$ .

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$\Rightarrow y_1, y_2, \dots, y_n$  are independent  $y_i \sim \mathcal{N}(a + b \cdot x_i, \sigma^2)$ .

$a, b, \sigma^2$  are unknown, but **not random**.

We estimate  $a$  and  $b$  by computing

$$(\hat{a}, \hat{b}) := \arg \min_{(a,b)} \sum_i (y_i - (a + b \cdot x_i))^2.$$

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## Theorem

Compute  $\hat{a}$  and  $\hat{b}$  by

$$\hat{b} = \frac{\sum_i (y_i - \bar{y}) \cdot (x_i - \bar{x})}{\sum_i (x_i - \bar{x})^2} = \frac{\sum_i y_i \cdot (x_i - \bar{x})}{\sum_i (x_i - \bar{x})^2}$$

and

$$\hat{a} = \bar{y} - \hat{b} \cdot \bar{x}.$$

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and

$$\hat{a} = \bar{y} - \hat{b} \cdot \bar{x}.$$

### Please keep in mind:

The line  $y = \hat{a} + \hat{b} \cdot x$  goes through the center of gravity of the cloud of points  $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$ .

vulture

	day	heartbpm	metabol	minTemp	maxTemp	medtemp
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.	.	.	.	.	.	.
.	.	.	.	.	.	.
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(14 different days)

```

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> summary(model)
Call:
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Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1 1
Residual standard error: 0.912 on 17 degrees of freedom
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F-statistic: 529.7 on 1 and 17 DF,  p-value: 2.979e-14

```

# Optimizing clutch sizes

Example: *Cowpea weevil* (also *bruchid beetle*)

*Callosobruchus maculatus*

German: Erbsensamenkäfer



Wilson, K. (1994) Evolution of clutch size in insects. II. A test of static optimality models using the beetle *Callosobruchus maculatus* (Coleoptera: Bruchidae).

*Journal of Evolutionary Biology* **7**: 365–386.

How does survival probability depend on clutch size?



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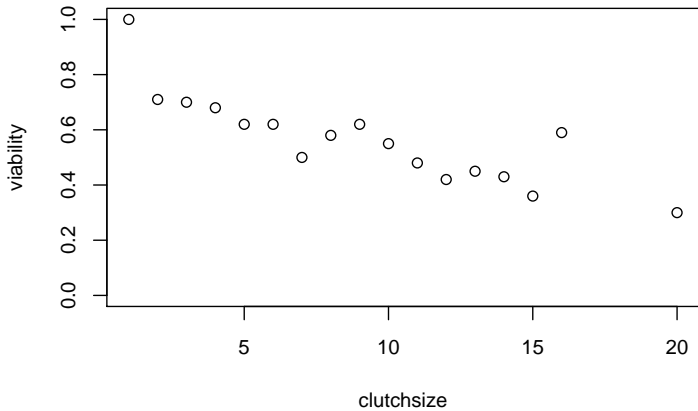


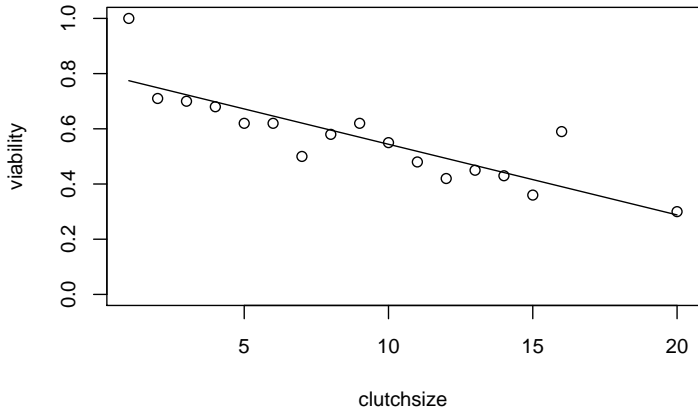
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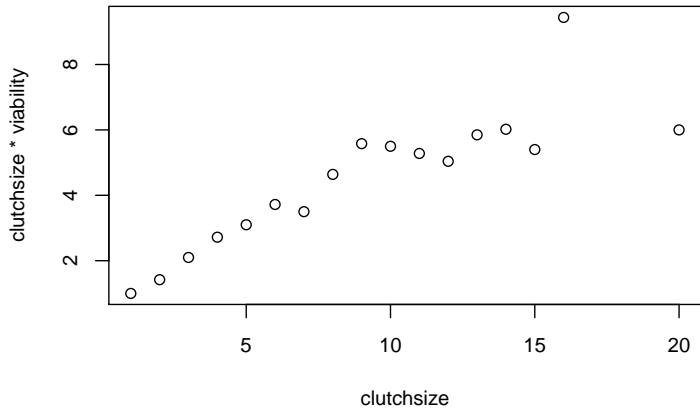
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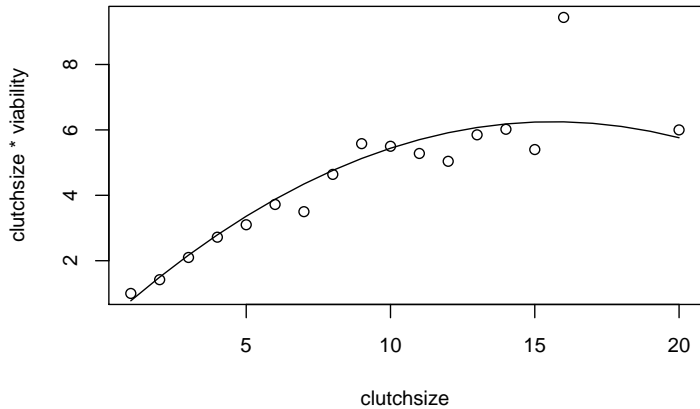
How does survival probability depend on clutch size?

Which clutch size optimizes the expected number of surviving offspring?









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## Example: red deer (*Cervus elaphus*)

theory: femals can influence the sex of their offspring

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theory: femals can influence the sex of their offspring

Evolutionary stable strategy: weak animals may tend to have female offspring, strong animals may tend to have male offspring.



Clutton-Brock, T. H. , Albon, S. D., Guinness, F. E. (1986)  
Great expectations: dominance, breeding success and  
offspring sex ratios in red deer.  
*Anim. Behav.* **34**, 460-471.

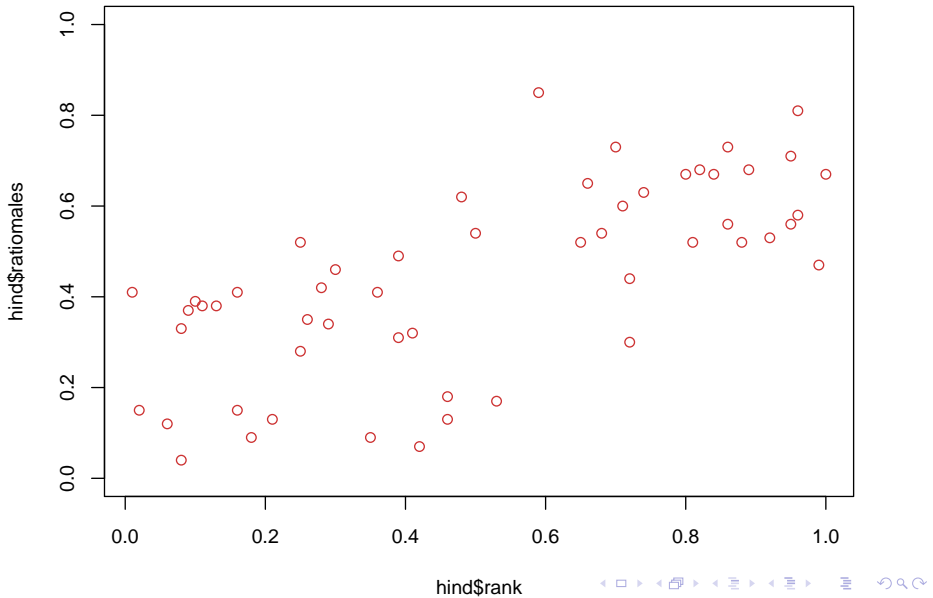


```
> hind
   rank ratiomales
1  0.01      0.41
2  0.02      0.15
3  0.06      0.12
4  0.08      0.04
5  0.08      0.33
6  0.09      0.37
.   .         .
.   .         .
.   .         .

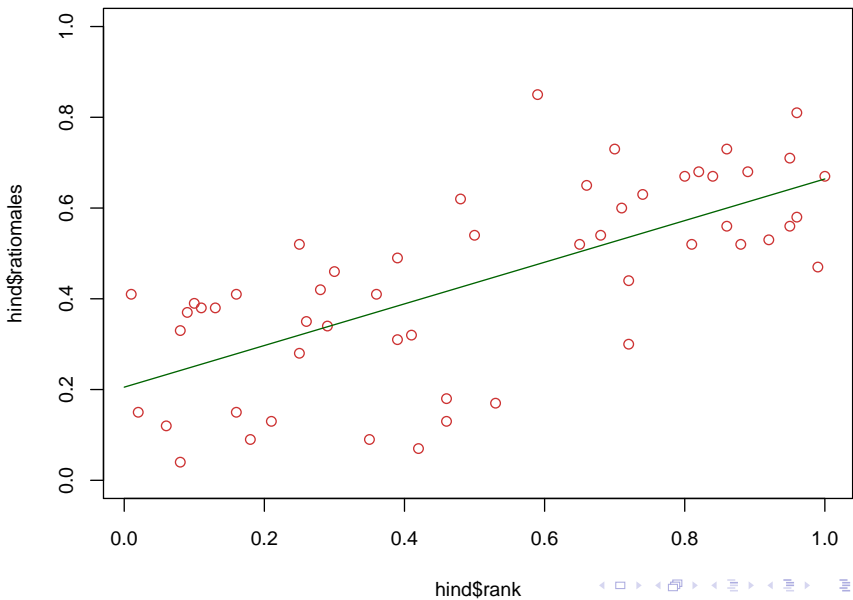
52 0.96      0.81
53 0.99      0.47
54 1.00      0.67
```

**CAUTION: Simulated data,  
inspired by original paper**

# t-test for linear regression



# t-test for linear regression



```
> mod <- lm(ratiomales~rank,data=hind)
```

```
> summary(mod)
```

```
Call:
```

```
lm(formula = ratiomales ~ rank, data = hind)
```

```
Residuals:
```

	Min	1Q	Median	3Q	Max
	-0.32798	-0.09396	0.02408	0.11275	0.37403

```
Coefficients:
```

	Estimate	Std. Error	t value	Pr(> t )	
(Intercept)	0.20529	0.04011	5.119	4.54e-06	***
rank	0.45877	0.06732	6.814	9.78e-09	***

```
---
```

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

```
Residual standard error: 0.154 on 52 degrees of freedom
```

```
Multiple R-squared: 0.4717, Adjusted R-squared: 0.4616
```

```
F-statistic: 46.44 on 1 and 52 DF, p-value: 9.78e-09
```

Model:

$$Y = a + b \cdot X + \varepsilon \quad \text{mit } \varepsilon \sim \mathcal{N}(0, \sigma^2)$$

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In other words: How can we test the null hypothesis  $b = 0$ ?

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How to compute the significance of a relationship between the *explanatory trait*  $X$  and the *target variable*  $Y$ ?

In other words: How can we test the null hypothesis  $b = 0$ ?

We have estimated  $b$  by  $\hat{b} \neq 0$ . Could the true  $b$  be 0?



Model:

$$Y = a + b \cdot X + \varepsilon \quad \text{mit } \varepsilon \sim \mathcal{N}(0, \sigma^2)$$

How to compute the significance of a relationship between the *explanatory trait*  $X$  and the *target variable*  $Y$ ?

In other words: How can we test the null hypothesis  $b = 0$ ?

We have estimated  $b$  by  $\hat{b} \neq 0$ . Could the true  $b$  be 0?

How large is the standard error of  $\hat{b}$ ?

# t-test for $\hat{b}$

Estimate  $\sigma^2$  by

$$s^2 = \frac{\sum_i (y_i - \hat{a} - \hat{b} \cdot x_i)^2}{n - 2}.$$

Then,

$$\frac{\hat{b} - b}{s / \sqrt{\sum_i (x_i - \bar{x})^2}}$$

is t-distributed with  $n - 2$  degrees of freedom. Thus, we can apply a t-test to test the null-hypothesis  $b = 0$ .

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- root of numbers of inhabitants and deaths

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- Example: Success of different therapies

- Example: Daphnia

Cross validation and AIC

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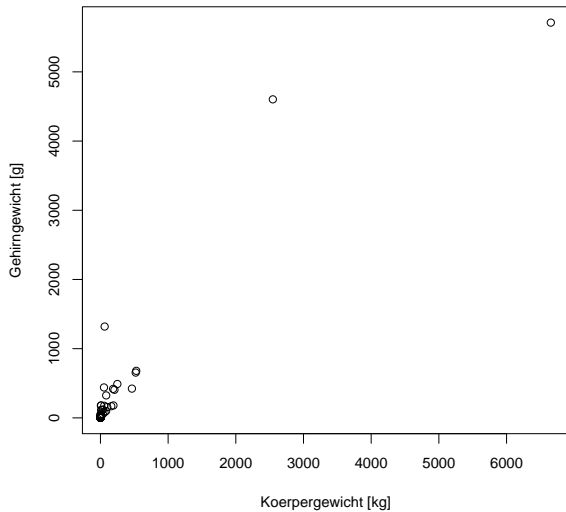
Cross validation and AIC

# Data example: typical body weight [kg] and and brain weight [g] of 62 mammals species (and 3 dinosaurs)

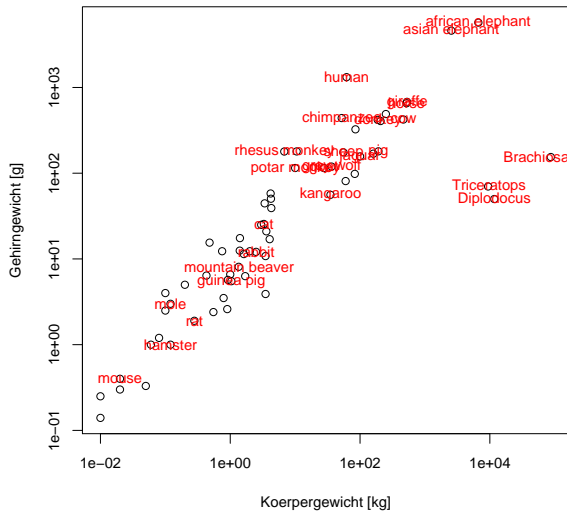
```
> data
```

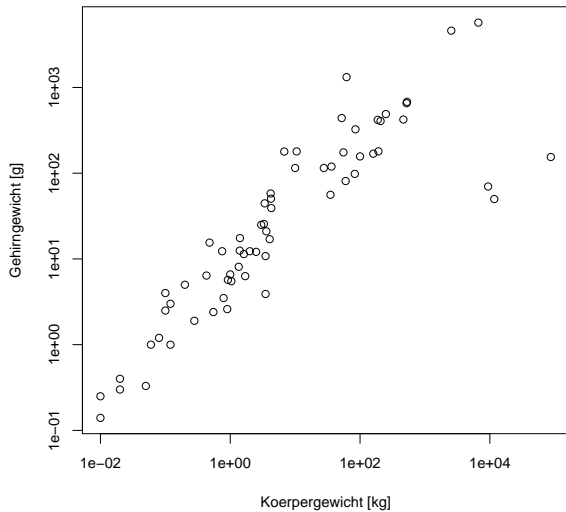
	weight.kg.	brain.weight.g	species	extinct
1	6654.00	5712.00	african elephant	no
2	1.00	6.60		no
3	3.39	44.50		no
4	0.92	5.70		no
5	2547.00	4603.00	asian elephant	no
6	10.55	179.50		no
7	0.02	0.30		no
8	160.00	169.00		no
9	3.30	25.60	cat	no
10	52.16	440.00	chimpanzee	no
11	0.43	6.40		
.	.	.	.	
.	.	.	.	
.	.	.	.	

## typische Werte bei 62 Saeugeierarten



## typische Werte bei 65 Saeugeierarten



**typische Werte bei 65 Saeugeierarten**



```
> modell <- lm(brain.weight.g~weight.kg.,subset=extinct=="no")
> summary(modell)
```

Call:

```
lm(formula = brain.weight.g ~ weight.kg., subset = extinct ==
    "no")
```

Residuals:

Min	1Q	Median	3Q	Max
-809.95	-87.43	-78.55	-31.17	2051.05

Coefficients:

	Estimate	Std. Error	t value	Pr(> t )
(Intercept)	89.91213	43.58134	2.063	0.0434 *
weight.kg.	0.96664	0.04769	20.269	<2e-16 ***

---

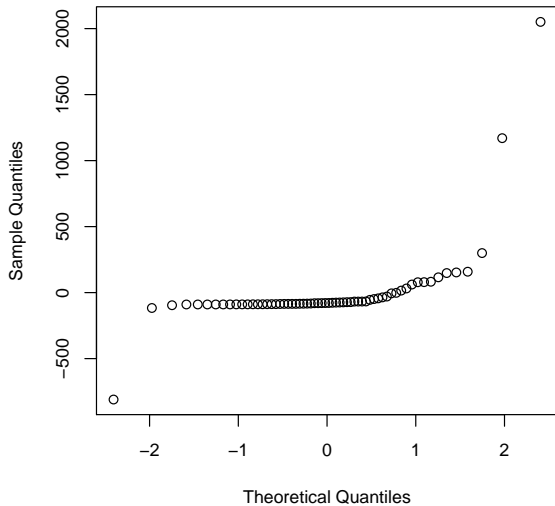
Signif. codes: 0 \*\*\* 0.001 \*\* 0.01 \* 0.05 . 0.1 1

Residual standard error: 334.8 on 60 degrees of freedom

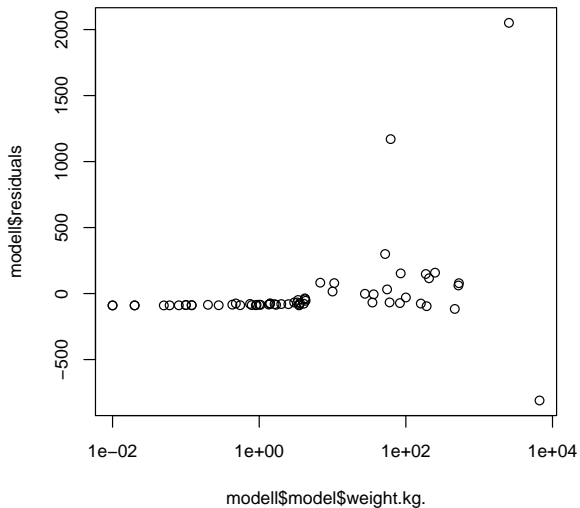
Multiple R-squared: 0.8726, Adjusted R-squared: 0.8704

F-statistic: 410.8 on 1 and 60 DF, p-value: < 2.2e-16

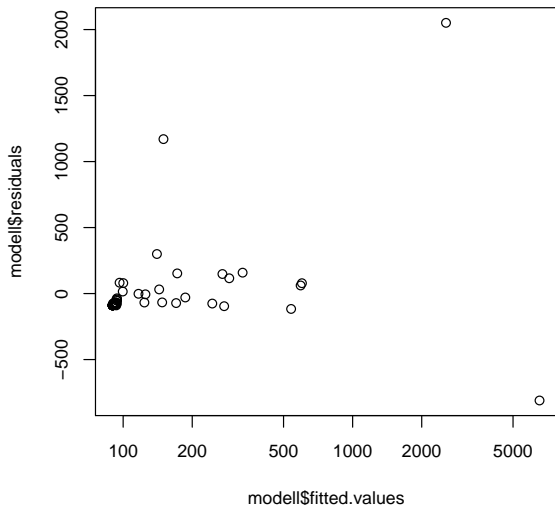
```
qqnorm(modell$residuals)
```

**Normal Q-Q Plot**

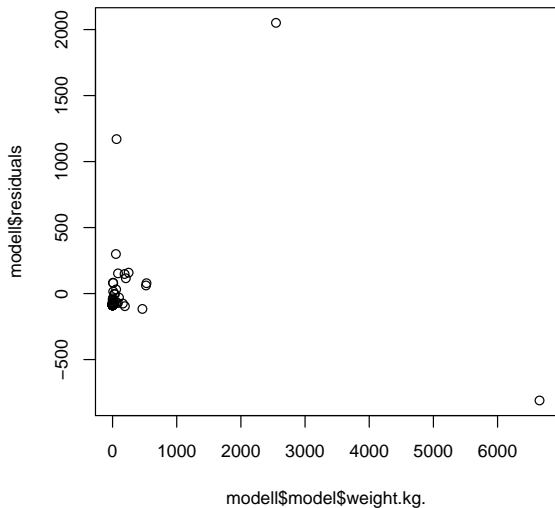
```
plot(modell$fitted.values,modell$residuals)
```



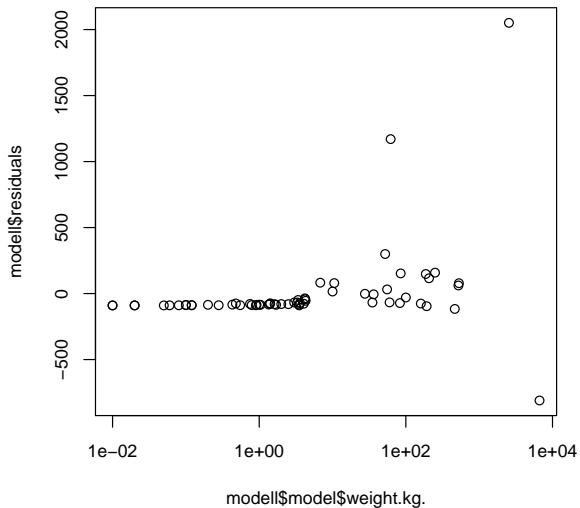
```
plot(modell$fitted.values,modell$residuals,log='x')
```



```
plot(modell$model$weight.kg.,modell$residuals)
```



```
plot(modell$model$weight.kg.,modell$residuals,log='x' )
```



We see that the residuals' variance depends on the fitted values (or the body weight): “heteroscedasticity”

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The model assumes *homoscedasticity*, i.e. the random deviations must be (almost) independent of the explaining traits (body weight) and the fitted values.



We see that the residuals' variance depends on the fitted values (or the body weight): “heteroscedasticity”

The model assumes *homoscedasticity*, i.e. the random deviations must be (almost) independent of the explaining traits (body weight) and the fitted values.

**variance-stabilizing transformation:**

can be rescale body- and brain size to make deviations independent of variables

Actually not so surprising: An elephant's brain of typically 5 kg can easily be 500 g lighter or heavier from individual to individual. This can not happen for a mouse brain of typically 5 g. The latter will rather also vary by 10%, i.e. 0.5 g. Thus, the variance is not additive but rather multiplicative:

$$\text{brain mass} = (\text{expected brain mass}) \cdot \text{random}$$

We can convert this into something with additive randomness by taking the log:

$$\log(\text{brain mass}) = \log(\text{expected brain mass}) + \log(\text{random})$$

```
> logmodell <- lm(log(brain.weight.g)~log(weight.kg.),subset=
> summary(logmodell)
```

Call:

```
lm(formula = log(brain.weight.g) ~ log(weight.kg.), subset = c
    "no")
```

Residuals:

Min	1Q	Median	3Q	Max
-1.68908	-0.51262	-0.05016	0.46023	1.97997

Coefficients:

	Estimate	Std. Error	t value	Pr(> t )
(Intercept)	2.11067	0.09794	21.55	<2e-16 ***
log(weight.kg.)	0.74985	0.02888	25.97	<2e-16 ***

---

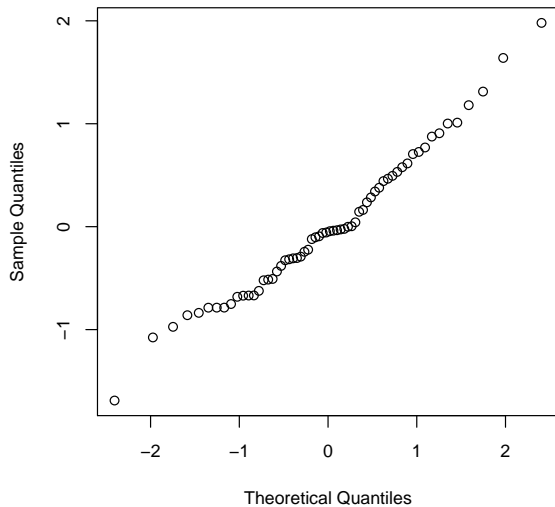
Signif. codes: 0 \*\*\* 0.001 \*\* 0.01 \* 0.05 . 0.1 1

Residual standard error: 0.7052 on 60 degrees of freedom

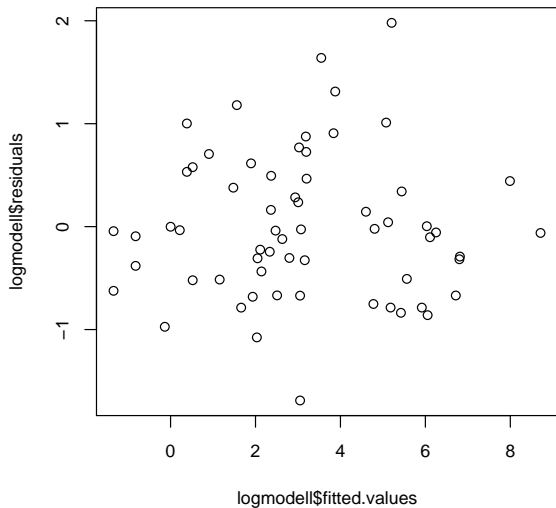
Multiple R-squared: 0.9183, Adjusted R-squared: 0.9169

F-statistic: 674.3 on 1 and 60 DF. p-value: < 2.2e-16

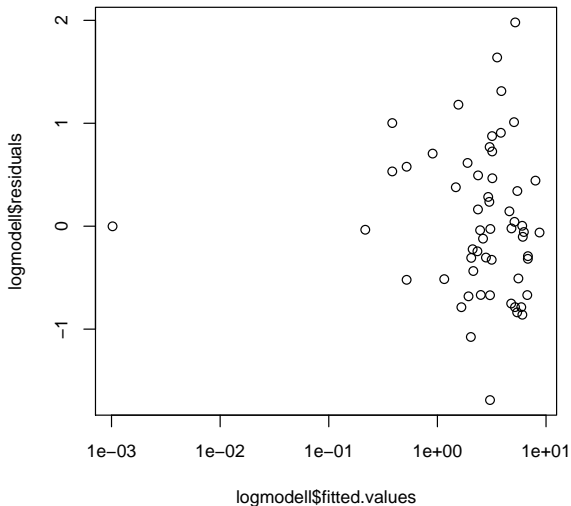
```
qqnorm(modell$residuals)
```

**Normal Q-Q Plot**

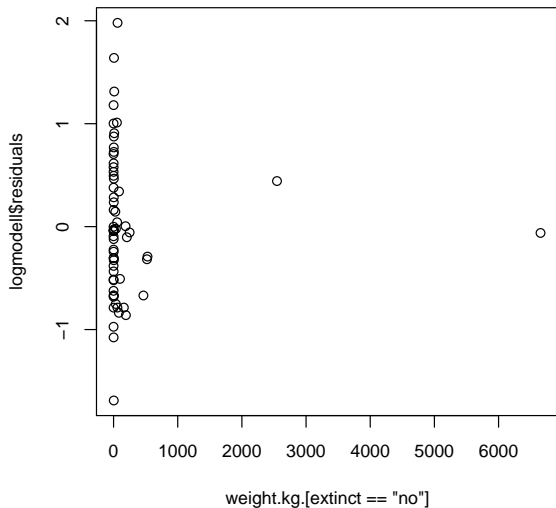
```
plot(logmodell$fitted.values, logmodell$residuals)
```



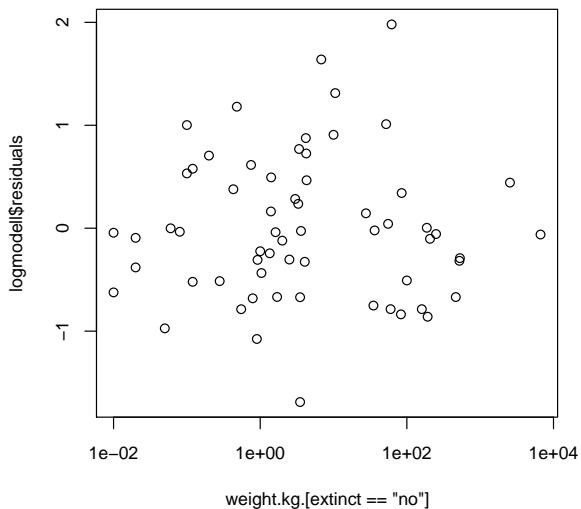
```
plot(logmodell$fitted.values, logmodell$residuals, log='x'  
)
```



```
plot(weight.kg.[extinct=='no'], logmodel$residuals)
```



```
plot(weight.kg.[extinct='no'], logmodel1$residuals, log='x',  
)
```





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## Cross validation and AIC

Data: For 301 US-american (Counties) number of white female inhabitants from 1960 and number of deaths by breast cancer in this group between 1950 and 1960. (Rice (2007) Mathematical Statistics and Data Analysis.)

```
> canc
      deaths inhabitants
1         1         445
2         0         559
3         3         677
4         4         681
5         3         746
6         4         869
.         .           .
.         .           .
.         .           .

300     248       74005
301     360       88456
```

Is the average number of deaths proportional to population size, i.e.

$$\mathbb{E} \text{deaths} = b \cdot \text{inhabitants}$$

or does the cancer risk depend on the size of the county, such that a different model fits better? e.g.

$$\mathbb{E} \text{deaths} = a + b \cdot \text{inhabitants}$$

with  $a \neq 0$ .

```
> modell <- lm(deaths~inhabitants,data=canc)
> summary(modell)
Call:
lm(formula = deaths ~ inhabitants, data = canc)
Residuals:
      Min       1Q   Median       3Q      Max
-66.0215  -4.1279   0.6769   5.2357  87.2989
Coefficients:
              Estimate Std. Error t value Pr(>|t|)
(Intercept) -5.261e-01  9.692e-01  -0.543   0.588
inhabitants  3.578e-03  5.446e-05  65.686  <2e-16 ***
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1 1
Residual standard error: 13 on 299 degrees of freedom
Multiple R-squared:  0.9352, Adjusted R-squared:  0.935
F-statistic:  4315 on 1 and 299 DF,  p-value: < 2.2e-16
```

The intercept is estimated to  $-0.526$ , but not significantly different from 0.

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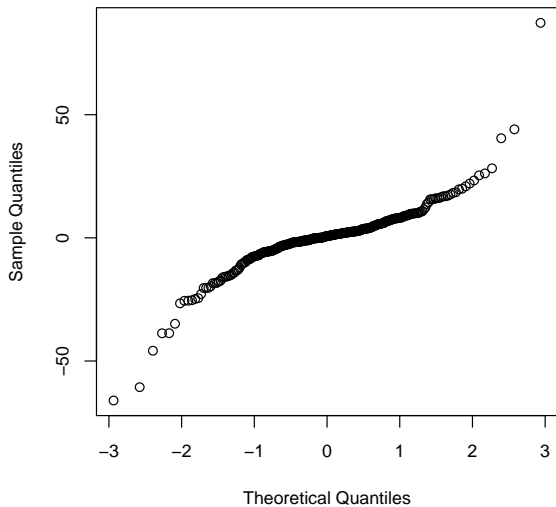
Thus we cannot reject the null hypothesis that the county size has no influence on the cancer risk.

The intercept is estimated to  $-0.526$ , but not significantly different from 0.

Thus we cannot reject the null hypothesis that the county size has no influence on the cancer risk.

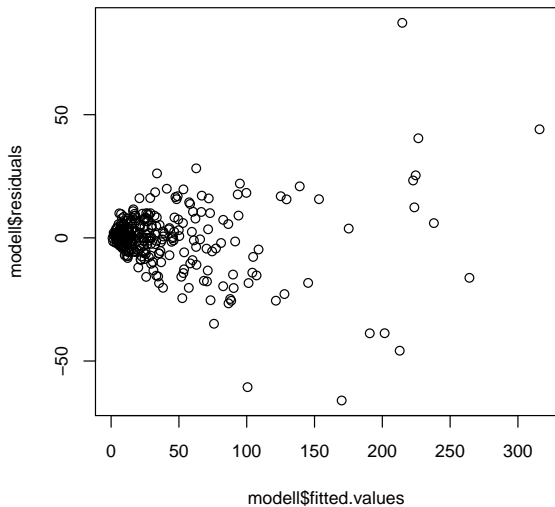
But.. does the model fit?

```
qqnorm(modell$residuals)
```

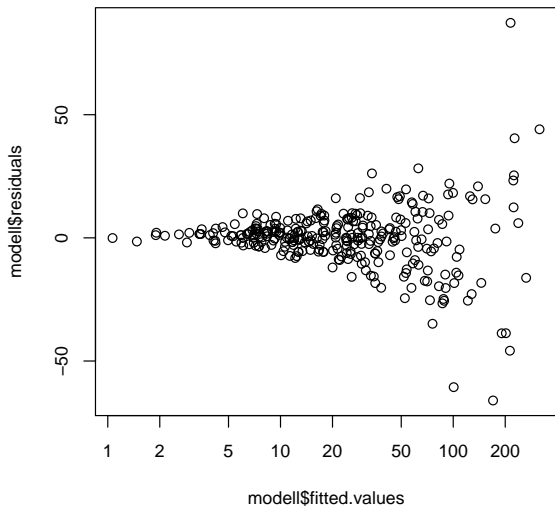
**Normal Q-Q Plot**



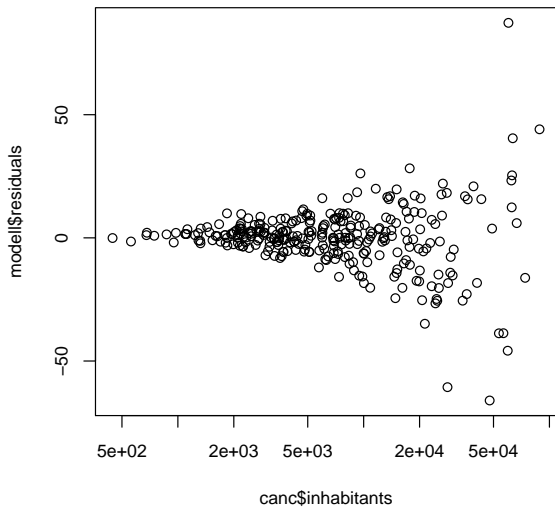
```
plot(modell$fitted.values,modell$residuals)
```



```
plot(modell$fitted.values,modell$residuals,log='x')
```



```
plot(canc$inhabitants,modell$residuals,log='x')
```



The variance of the residuals depends on the fitted values.  
*Heteroscedasticity*

The variance of the residuals depends on the fitted values.

*Heteroscedasticity*

The linear model assumes *Homoscedasticity*.

The variance of the residuals depends on the fitted values.

*Heteroscedasticity*

The linear model assumes *Homoscedasticity*.

**Variance Stabilizing Transformation:**

How can we rescale the population size such that we obtain homoscedastic data?

Where does the variance come from?

Where does the variance come from?

If  $n$  is the number of white female inhabitants and  $p$  the individual probability to die by breast cancer within 10 years, then  $np$  is the expected number of deaths and the variance is

$$n \cdot p \cdot (1 - p) \approx n \cdot p$$

(Maybe approximate binomial by Poisson). Standard deviation:  
 $\sqrt{n \cdot p}$ .



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$$n \cdot p \cdot (1 - p) \approx n \cdot p$$

(Maybe approximate binomial by Poisson). Standard deviation:  
 $\sqrt{n \cdot p}$ .

In this case we can approximately stabilize variance by taking the root on both sides of the equation.

Explanation:

$$\sqrt{y} = b \cdot \sqrt{x} + \varepsilon$$

$$\begin{aligned} \Rightarrow y &= (b \cdot \sqrt{x} + \varepsilon)^2 \\ &= b^2 \cdot x + 2 \cdot b \cdot \sqrt{x} \cdot \varepsilon + \varepsilon^2 \end{aligned}$$

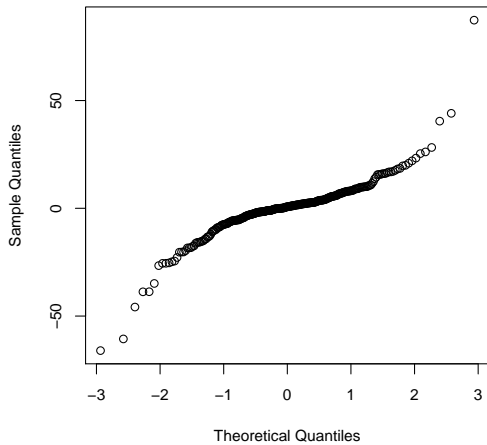
SD is not exactly proportional to  $\sqrt{x}$ , but at least  $2 \cdot b \cdot \sqrt{x} \cdot \varepsilon$  has SD prop. to  $\sqrt{x}$ , namely  $2 \cdot b \cdot \sqrt{x} \cdot \sigma$ . The Term  $\varepsilon^2$  is the  $\sigma^2$ -fold of a  $\chi_1^2$ -distributed random variable and has  $\text{SD} = \sigma^2 \cdot \sqrt{2}$ . If  $\sigma$  is small compared to  $b \cdot \sqrt{x}$ , the approximation

$$y \approx b^2 \cdot x + 2 \cdot b \cdot \sqrt{x} \cdot \varepsilon$$

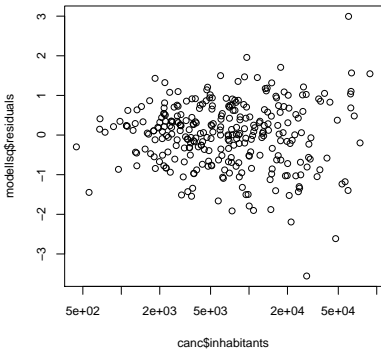
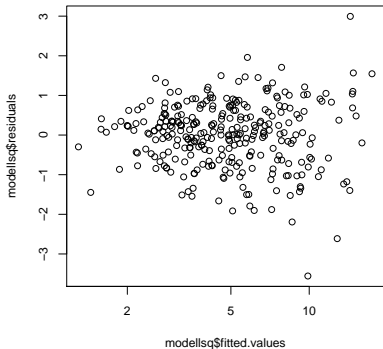
is reasonable and the SD of  $y$  is approximately proportional to  $\sqrt{x}$ .

```
> modellsq <- lm(sqrt(deaths)~sqrt(inhabitants),data=canc)
> summary(modellsq)
Call:
lm(formula = sqrt(deaths) ~ sqrt(inhabitants), data = canc)
Residuals:
    Min       1Q   Median       3Q      Max
-3.55639 -0.51900  0.06204  0.54277  2.99434
Coefficients:
                Estimate Std. Error t value Pr(>|t|)
(Intercept)    0.0664320  0.0974338   0.682   0.496
sqrt(inhabitants) 0.0583722  0.0009171  63.651 <2e-16 ***
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1 1
Residual standard error: 0.8217 on 299 degrees of freedom
Multiple R-squared:  0.9313, Adjusted R-squared:  0.931
F-statistic:  4051 on 1 and 299 DF,  p-value: < 2.2e-16
```

```
qqnorm(modell$residuals)
```

**Normal Q-Q Plot**

```
plot(modellsq$fitted.values,modellsq$residuals,log='x')  
plot(canc$inhabitants,modellsq$residuals,log='x')
```



The qqnorm plot is not perfect by at least the variance is stabilized.

The qqnorm plot is not perfect by at least the variance is stabilized.

The result remains the same: No significant relation between county size and breast cancer death risk.

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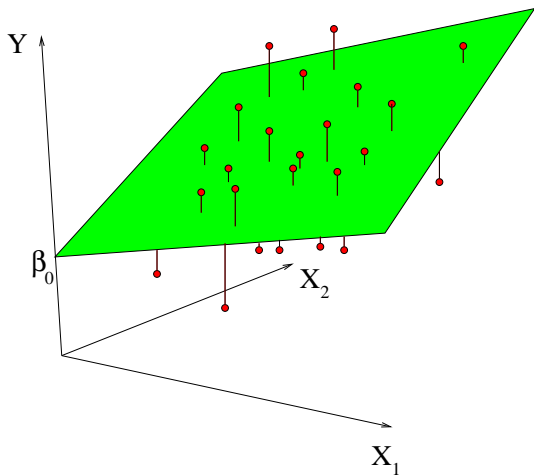
Example: Success of different therapies

Example: Daphnia

Cross validation and AIC



# Multivariate Regression



# Multivariate Regression

Problem: Predict  $Y$  from  $X_1, X_2, \dots, X_m$ .

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Observations:

$$Y_1 \quad , \quad X_{11}, X_{21}, \dots, X_{m1}$$

$$Y_2 \quad , \quad X_{12}, X_{22}, \dots, X_{m2}$$

$$\vdots \quad \quad \quad \vdots$$

$$Y_n \quad , \quad X_{1n}, X_{2n}, \dots, X_{mn}$$

# Multivariate Regression

Problem: Predict  $Y$  from  $X_1, X_2, \dots, X_m$ .

Observations:

$$Y_1, X_{11}, X_{21}, \dots, X_{m1}$$

$$Y_2, X_{12}, X_{22}, \dots, X_{m2}$$

$$\vdots$$

$$Y_n, X_{1n}, X_{2n}, \dots, X_{mn}$$

Model:  $Y = a + b_1 \cdot X_1 + b_2 \cdot X_2 + \dots + b_m \cdot X_m + \varepsilon$

# Multivariate Regression

Problem: Predict  $Y$  from  $X_1, X_2, \dots, X_m$ .

Observations:

$$\begin{array}{l} Y_1, X_{11}, X_{21}, \dots, X_{m1} \\ Y_2, X_{12}, X_{22}, \dots, X_{m2} \\ \vdots \\ Y_n, X_{1n}, X_{2n}, \dots, X_{mn} \end{array}$$

Model:  $Y = a + b_1 \cdot X_1 + b_2 \cdot X_2 + \dots + b_m \cdot X_m + \varepsilon$

Equation system to determine  $a, b_1, b_2, \dots, b_m$ :

$$\begin{array}{l} Y_1 = a + b_1 \cdot X_{11} + b_2 \cdot X_{21} + \dots + b_m \cdot X_{m1} + \varepsilon_1 \\ Y_2 = a + b_1 \cdot X_{12} + b_2 \cdot X_{22} + \dots + b_m \cdot X_{m2} + \varepsilon_2 \\ \vdots \\ Y_n = a + b_1 \cdot X_{1n} + b_2 \cdot X_{2n} + \dots + b_m \cdot X_{mn} + \varepsilon_n \end{array}$$

Model:

$$\begin{array}{rcccccccccccc}
 Y_1 & = & a & + & b_1 \cdot X_{11} & + & b_2 \cdot X_{21} & + & \dots & + & b_m \cdot X_{m1} & + & \varepsilon_1 \\
 Y_2 & = & a & + & b_1 \cdot X_{12} & + & b_2 \cdot X_{22} & + & \dots & + & b_m \cdot X_{m2} & + & \varepsilon_2 \\
 \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\
 Y_n & = & a & + & b_1 \cdot X_{1n} & + & b_n \cdot X_{2n} & + & \dots & + & b_m \cdot X_{mn} & + & \varepsilon_n
 \end{array}$$

target variable  $Y$

explanatory variables  $X_1, X_2, \dots, X_m$

parameter to be estimated  $a, b_1, \dots, b_m$

independent normally distributed perturbations  $\varepsilon_1, \dots, \varepsilon_m$  with unknown variance  $\sigma^2$ .

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**Example: species richness on sandy beaches**

Example: Success of different therapies

Example: Daphnia

Cross validation and AIC

- ▶ Which factors influence the species richness on sandy beaches?
- ▶ Data from the dutch National Institute for Coastal and Marine Management Rijkswaterstaat/RIKZ
- ▶ see also



Zuur, Ieno, Smith (2007) *Analysing Ecological Data*.  
Springer



	richness	angle2	NAP	grainsize	humus	week
1	11	96	0.045	222.5	0.05	1
2	10	96	-1.036	200.0	0.30	1
3	13	96	-1.336	194.5	0.10	1
4	11	96	0.616	221.0	0.15	1
.	.	.	.	.	.	.
.	.	.	.	.	.	.
21	3	21	1.117	251.5	0.00	4
22	22	21	-0.503	265.0	0.00	4
23	6	21	0.729	275.5	0.10	4
.	.	.	.	.	.	.
.	.	.	.	.	.	.
43	3	96	-0.002	223.0	0.00	3
44	0	96	2.255	186.0	0.05	3
45	2	96	0.865	189.5	0.00	3

# Meaning of the Variables

**richness** Number of species that were found in a plot.

**angle2** slope of the beach at the plot

**NAP** altitude of the plot compared to the mean sea level.

**grainsize** average diameter of sand grains

**humus** fraction of organic material

**week** in which of 4 was this plot probed.

(many more variables in original data set)

Model 0:

$$\text{richness} = a + b_1 \cdot \text{angle2} + b_2 \cdot \text{NAP} + b_3 \cdot \text{grainsize} + b_4 \cdot \text{humus} + \varepsilon$$

Model 0:

$$\text{richness} = a + b_1 \cdot \text{angle2} + b_2 \cdot \text{NAP} + b_3 \cdot \text{grainsize} + b_4 \cdot \text{humus} + \varepsilon$$

in R notation:

```
richness ~ angle2 + NAP + grainsize + humus
```

```
> modell0 <- lm(richness ~ angle2+NAP+grainsize+humus,  
+               data = rikz)
```

```
> summary(modell0)
```

Call:

```
lm(formula = richness ~ angle2 + NAP + grainsize + humus, data = rikz)
```

Residuals:

Min	1Q	Median	3Q	Max
-4.6851	-2.1935	-0.4218	1.6753	13.2957

Coefficients:

	Estimate	Std. Error	t value	Pr(> t )	
(Intercept)	18.35322	5.71888	3.209	0.00262	**
angle2	-0.02277	0.02995	-0.760	0.45144	
NAP	-2.90451	0.59068	-4.917	1.54e-05	***
grainsize	-0.04012	0.01532	-2.619	0.01239	*
humus	11.77641	9.71057	1.213	0.23234	

---

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

Residual standard error: 3.644 on 40 degrees of freedom

Multiple R-squared: 0.5178. Adjusted R-squared: 0.4696

- ▶ e.g. -2.90451 is the estimator for  $b_2$ , the coefficient of NAP

- ▶ e.g. -2.90451 is the estimator for  $b_2$ , the coefficient of NAP
- ▶ The  $p$  value  $\Pr(>|t|)$  refers to the null hypothesis that the true parameter value may be 0, i.e. the (potentially) explanatory variable (e.g. NAP) has actually no effect on the target variable (the species richness).

- ▶ e.g. -2.90451 is the estimator for  $b_2$ , the coefficient of NAP
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- ▶ NAP is judged to be highly significant, grainsize also.
- ▶ Is there a significant week effect?
- ▶ Not the number 1,2,3,4 of the week should be multiplied with a coefficient. Instead, the numbers are taken as a non-numerical factor, i.e. each of the weeks 2,3,4 get a parameter that describes how much the species richness is increased compared to week 1.

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- ▶ In R this is done by changing `week` into a factor.

## Model 0:

$$\begin{aligned} \text{richness} = & a + b_1 \cdot \text{angle2} + b_2 \cdot \text{NAP} + b_3 \cdot \text{grainsize} + \\ & + b_4 \cdot \text{humus} + \\ & b_5 \cdot I_{\text{week}=2} + b_6 \cdot I_{\text{week}=3} + b_7 \cdot I_{\text{week}=4} + \varepsilon \end{aligned}$$

$I_{\text{week}=k}$  is a so-called indicator variable which is 1 if  $\text{week}=k$  and 0 otherwise.

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e.g.  $b_7$  describes, by how much the species richness in an average plot probed in week 3 is increased compared to week 1.

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$I_{\text{week}=k}$  is a so-called indicator variable which is 1 if  $\text{week}=k$  and 0 otherwise.

e.g.  $b_7$  describes, by how much the species richness in an average plot probed in week 3 is increased compared to week 1.

in R notation:

```
richness ~ angle2 + NAP + grainsize + humus +  
factor(week)
```

```
> modell <- lm(richness ~ angle2+NAP+grainsize+humus
+               +factor(week), data = rikz)
> summary(modell)
```

```
.
.
.
```

Coefficients:

	Estimate	Std. Error	t value	Pr(> t )	
(Intercept)	9.298448	7.967002	1.167	0.250629	
angle2	0.016760	0.042934	0.390	0.698496	
NAP	-2.274093	0.529411	-4.296	0.000121	***
grainsize	0.002249	0.021066	0.107	0.915570	
humus	0.519686	8.703910	0.060	0.952710	
factor(week)2	-7.065098	1.761492	-4.011	0.000282	***
factor(week)3	-5.719055	1.827616	-3.129	0.003411	**
factor(week)4	-1.481816	2.720089	-0.545	0.589182	

- ▶ Obviously, in weeks 2 and 3 significantly less species were found than in week 1, which is our reference point here.



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- ▶ The estimated `Intercept` is thus the expected species richness in week 1 in a plot where all other parameters take the value 0.

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- ▶ The estimated `Intercept` is thus the expected species richness in week 1 in a plot where all other parameters take the value 0.
- ▶ An alternative representation without `Intercept` takes 0 as reference point.

```
> modell.alternativ <- lm(richness ~ angle2+NAP+
+       grainsize+humus+factor(week)-1, data = rikz)
> summary(modell.alternativ)
```

```
.
.
.
```

Coefficients:

	Estimate	Std. Error	t value	Pr(> t )	
angle2	0.016760	0.042934	0.390	0.698496	
NAP	-2.274093	0.529411	-4.296	0.000121	***
grainsize	0.002249	0.021066	0.107	0.915570	
humus	0.519686	8.703910	0.060	0.952710	
factor(week)1	9.298448	7.967002	1.167	0.250629	
factor(week)2	2.233349	8.158816	0.274	0.785811	
factor(week)3	3.579393	8.530193	0.420	0.677194	
factor(week)4	7.816632	6.522282	1.198	0.238362	

the  $p$  values refer to the question whether the four intercepts for the different weeks are significantly different from 0.

The four  $p$  values refer to the null hypotheses that the additive parameter of a week is 0.

How do we test whether there is a difference between the weeks?

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If we perform pairwise test for the weeks, we end up with  $\binom{4}{2} = 6$  tests.

Bonferroni correction: Multiply each  $p$  value with the number of tests performed, in our case 6.

# Bonferroni correction

**Problem:** If you perform many tests, some of them will reject the null hypothesis even if the null hypothesis is true.

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- Example:** If you perform 20 tests where the null hypothesis is actually true, then on average 1 test will falsely reject the null hypothesis on the 5% level.

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**Example:** If you perform 20 tests where the null hypothesis is actually true, then on average 1 test will falsely reject the null hypothesis on the 5% level.

**Bonferroni correction:** Multiply all  $p$  values with the number of tests performed. Reject the null hypotheses where the result is still smaller than the significance level.

# Bonferroni correction

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**Example:** If you perform 20 tests where the null hypothesis is actually true, then on average 1 test will falsely reject the null hypothesis on the 5% level.

**Bonferroni correction:** Multiply all  $p$  values with the number of tests performed. Reject the null hypotheses where the result is still smaller than the significance level.

**Disadvantage:** Conservative: Often, the null hypotheses cannot be rejected even if it is not true (type-2-error).

Alternative: Test whether there is a week effect by using an analysis of variance (anova) to compare a model with week effect to a model without week effect.

Alternative: Test whether there is a week effect by using an analysis of variance (anova) to compare a model with week effect to a model without week effect.

Only works for nested models, i.e. the simpler model can be obtained by restricting some parameters of the richer model to certain values or equations. In our case: “all week summands are equal”.

```
> modell0 <- lm(richness ~ angle2+NAP+grainsize+humus,
+               data = rikz)
> modell <- lm(richness ~ angle2+NAP+grainsize+humus
+              +factor(week), data = rikz)
> anova(modell0, modell)
```

### Analysis of Variance Table

Model 1: richness ~ angle2 + NAP + grainsize + humus

Model 2: richness ~ angle2 + NAP + grainsize + humus + factor

	Res.Df	RSS	Df	Sum of Sq	F	Pr(>F)
1	40	531.17				
2	37	353.66	3	177.51	6.1902	0.00162 **

---

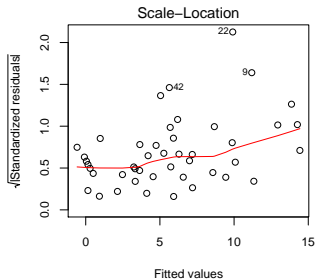
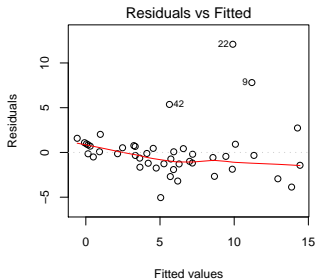
Signif. codes: 0 '\*\*\*' 0.001 '\*\*' 0.01 '\*' 0.05 '.' 0.1 ' ' 1



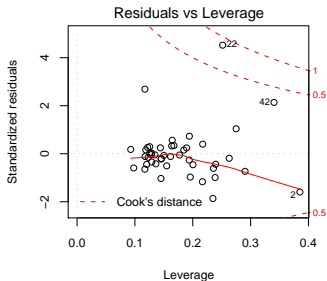
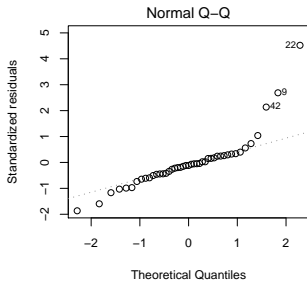
We reject the null hypothesis that the weeks have no effect with a  $p$ -value of 0.00162.

We reject the null hypothesis that the weeks have no effect with a  $p$ -value of 0.00162.

But wait! We can only do that if the more complex model fits well to the data. We check this graphically.



```
plot(modell)
```



Probes 22, 42, and 9 are considered as outliers.

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Can we explain this by taking more parameters into account or are these real outliers, which are atypical and must be analysed separately.

Is there an interaction between NAP and angle2?

Is there an interaction between NAP and angle2?

$$\begin{aligned} \text{richness} = & a + b_1 \cdot \text{angle2} + b_2 \cdot \text{NAP} + b_3 \cdot \text{grainsize} + \\ & + b_4 \cdot \text{humus} + \\ & + b_5 \cdot I_{\text{week}=2} + b_6 \cdot I_{\text{week}=3} + b_7 \cdot I_{\text{week}=4} \\ & + b_8 \cdot \text{angle2} \cdot \text{NAP} + \varepsilon \end{aligned}$$

in R notation:

```
richness ~ angle2 + NAP + angle2:NAP+grainsize + humus  
+ factor(week)
```

Is there an interaction between NAP and angle2?

$$\begin{aligned} \text{richness} = & a + b_1 \cdot \text{angle2} + b_2 \cdot \text{NAP} + b_3 \cdot \text{grainsize} + \\ & + b_4 \cdot \text{humus} + \\ & + b_5 \cdot I_{\text{week}=2} + b_6 \cdot I_{\text{week}=3} + b_7 \cdot I_{\text{week}=4} \\ & + b_8 \cdot \text{angle2} \cdot \text{NAP} + \varepsilon \end{aligned}$$

in R notation:

```
richness ~ angle2 + NAP + angle2:NAP+grainsize + humus
+ factor(week)
```

short-cut:

```
richness ~ angle2*NAP+grainsize + humus + factor(week)
```



```

> modell3 <- lm(richness ~ angle2*NAP+grainsize+humus
+               +factor(week), data = rikz)
> summary(modell3)
[...]
```

Coefficients:

	Estimate	Std. Error	t value	Pr(> t )	
(Intercept)	10.438985	8.148756	1.281	0.208366	
angle2	0.007846	0.044714	0.175	0.861697	
NAP	-3.011876	1.099885	-2.738	0.009539	**
grainsize	0.001109	0.021236	0.052	0.958658	
humus	0.387333	8.754526	0.044	0.964955	
factor(week)2	-7.444863	1.839364	-4.048	0.000262	***
factor(week)3	-6.052928	1.888789	-3.205	0.002831	**
factor(week)4	-1.854893	2.778334	-0.668	0.508629	
angle2:NAP	0.013255	0.017292	0.767	0.448337	

---

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

## Different types of ANOVA tables

If you apply the R command `anova` to a single model, the variables are added consecutively in the same order as in the command. Each  $p$  value refers to the test whether the model gets significantly better by adding the variable to only those that are listed above the variable. In contrast to this, the  $p$  values that are given by `summary` or by `dropterm` from the MASS library always compare the model to a model where only the corresponding variable is set to 0 and all other variables can take any values. The  $p$  values given by `anova` thus depend on the order in which the variables are given in the command. This is not the case for `summary` and `dropterm`. The same options exist in other software packages, sometimes under the names “type I analysis” and “type II analysis”.

The same model is specified twice:

```
> modellA <- lm(richness ~ angle2+NAP+humus
+               +factor(week)+grainsize,data = rikz)
> modellB <- lm(richness ~ angle2+grainsize
+               +NAP+humus+factor(week), data = rikz)
```

Look at the  $p$ -value of grainsize

```
> anova(modellA)
```

## Analysis of Variance Table

Response: richness

	Df	Sum Sq	Mean Sq	F value	Pr(>F)	
angle2	1	124.86	124.86	13.0631	0.0008911	***
NAP	1	319.32	319.32	33.4071	1.247e-06	***
humus	1	35.18	35.18	3.6804	0.0627983	.
factor(week)	3	268.51	89.50	9.3638	9.723e-05	***
grainsize	1	0.11	0.11	0.0114	0.9155704	
Residuals	37	353.66	9.56			

---

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

```
> anova(modellB)
```

```
Analysis of Variance Table
```

```
Response: richness
```

	Df	Sum Sq	Mean Sq	F value	Pr(>F)	
angle2	1	124.86	124.86	13.0631	0.00089	***
grainsize	1	35.97	35.97	3.7636	0.06003	.
NAP	1	390.11	390.11	40.8127	1.8e-07	***
humus	1	19.53	19.53	2.0433	0.16127	
factor(week)	3	177.51	59.17	6.1902	0.00162	**
Residuals	37	353.66	9.56			

```
---
```

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

```
> library(MASS)
> dropterm(modellA,test="F")
Single term deletions
```

Model:

```
richness ~ angle2 + NAP + humus + factor(week) + grainsize
              Df Sum of Sq    RSS    AIC  F Value      Pr(F)
<none>                353.66 108.78
angle2           1         1.46 355.12 106.96      0.15 0.6984
NAP              1       176.37 530.03 124.98     18.45 0.0001 ***
humus            1          0.03 353.70 106.78  0.003565 0.9527
factor(week)    3       177.51 531.17 121.08      6.19 0.0016 **
grainsize       1          0.11 353.77 106.79      0.01 0.9155
---
```

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

```
> dropterm(modellB, test="F")
```

```
Single term deletions
```

```
Model:
```

```
richness ~ angle2 + grainsize + NAP + humus + factor(week)
```

	Df	Sum of Sq	RSS	AIC	F Value	Pr(F)
<none>			353.66	108.78		
angle2	1	1.46	355.12	106.96	0.15	0.6984
grainsize	1	0.11	353.77	106.79	0.01	0.9155
NAP	1	176.37	530.03	124.98	18.45	0.0001 ***
humus	1	0.03	353.70	106.78	0.003565	0.9527
factor(week)	3	177.51	531.17	121.08	6.19	0.0016 **

```
---
```

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

```
> summary(modellA)
```

```
[...]
```

```
Coefficients:
```

	Estimate	Std. Error	t value	Pr(> t )	
(Intercept)	9.298448	7.967002	1.167	0.2506	
angle2	0.016760	0.042934	0.390	0.6984	
NAP	-2.274093	0.529411	-4.296	0.0001	***
humus	0.519686	8.703910	0.060	0.9527	
factor(week)2	-7.065098	1.761492	-4.011	0.0002	***
factor(week)3	-5.719055	1.827616	-3.129	0.0034	**
factor(week)4	-1.481816	2.720089	-0.545	0.5891	
grainsize	0.002249	0.021066	0.107	0.9155	

```
---
```

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



```
> summary(modellB)
```

```
[...]
```

```
Coefficients:
```

	Estimate	Std. Error	t value	Pr(> t )	
(Intercept)	9.298448	7.967002	1.167	0.2506	
angle2	0.016760	0.042934	0.390	0.6984	
grainsize	0.002249	0.021066	0.107	0.9155	
NAP	-2.274093	0.529411	-4.296	0.0001	***
humus	0.519686	8.703910	0.060	0.9527	
factor(week)2	-7.065098	1.761492	-4.011	0.0002	***
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```
---
```

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

# Contents

Regression toward the mean

Univariate linear regression: how and why?

t-test for linear regression

Examples with transformed variables

log-scaling brain sizes and body weights

root of numbers of inhabitants and deaths

**Multivariate Regression**

Example: species richness on sandy beaches

**Example: Success of different therapies**

Example: Daphnia

Cross validation and AIC

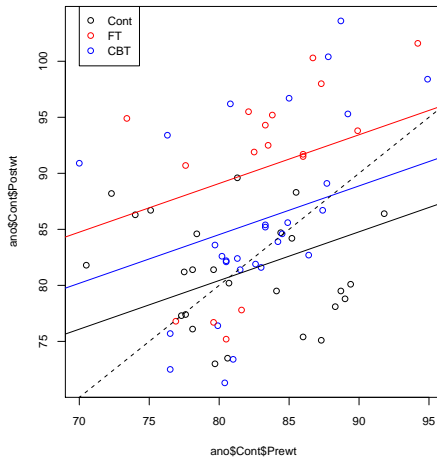
For young anorexia patients the effect of family therapy (FT) and cognitive behavioral therapy (CBT) is compared to a control group (Cont) by comparing the weight before (Prewt) and after (Postwt) the treatment (Treat).



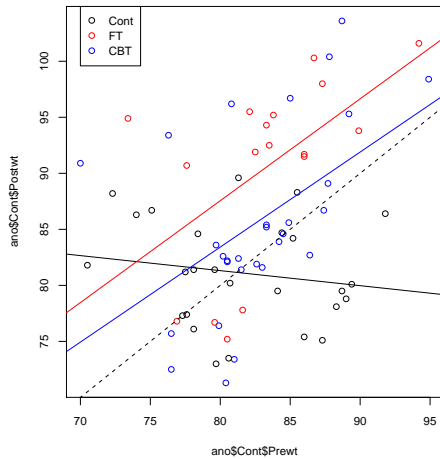
Hand, D. J., Daly, F., McConway, K., Lunn, D. and Ostrowski, E. eds (1993) *A Handbook of Small Data Sets*. Chapman & Hall

- Model Im1** There is a linear relation with the pre-weight. Each treatment changes the weight by a value that depends on the treatment but not on the treatment.
- Model Im2** Interaction between Treatment und Preweight: The effect of the pre-weight depends on the kind of treatment.

lm1



lm2



```
> lm1 <- lm(Postwt~Prewt+Treat,anorexia)
> lm2 <- lm(Postwt~Prewt*Treat,anorexia)
> anova(lm1,lm2)
```

### Analysis of Variance Table

Model 1: Postwt ~ Prewt + Treat

Model 2: Postwt ~ Prewt \* Treat

	Res.Df	RSS	Df	Sum of Sq	F	Pr(>F)
1	68	3311.3				
2	66	2844.8	2	466.5	5.4112	0.006666 **

---

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

**result:** the more complex model fits significantly better than the nested model.

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**interpretation:** The role of the weight before the treatment depends on the type of the treatment.



**result:** the more complex model fits significantly better than the nested model.

**interpretation:** The role of the weight before the treatment depends on the type of the treatment.  
or: The difference between effects of the treatments depends on the weight before the treatment.

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Question: Is there a difference between *Daphnia magna* and *Daphnia galeata* in their reaction on food supply?

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Data from Justina Wolinska's ecology course for Bachelor students.

```
> daph <- read.table("daphnia_justina.csv",h=T)
```

```
> daph
```

	counts	foodlevel	species
1	68	high	magna
2	54	high	magna
3	59	high	magna
4	24	high	galeata
5	27	high	galeata
6	16	high	galeata
7	20	low	magna
8	18	low	magna
9	18	low	magna
10	5	low	galeata
11	8	low	galeata
12	9	low	galeata

```
> mod1 <- lm(counts~foodlevel+species,data=daph)
> mod2 <- lm(counts~foodlevel*species,data=daph)
> anova(mod1,mod2)
```

### Analysis of Variance Table

Model 1: counts ~ foodlevel + species

Model 2: counts ~ foodlevel \* species

	Res.Df	RSS	Df	Sum of Sq	F	Pr(>F)
1	9	710.00				
2	8	176.67	1	533.33	24.151	0.001172 **

---

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

```
> summary(mod2)
```

```
[...]
```

```
Coefficients:
```

	Estimate	Std.Error	t.value	Pr(> t )	
(Intercept)	22.33	2.713	8.232	3.55e-05	***
countslow	-15.00	3.837	-3.909	0.00449	**
foodlevelmagna	38.00	3.837	9.904	9.12e-06	***
countslow:foodlevelmagna	-26.67	5.426	-4.914	0.00117	**

```
---
```

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

```
Residual standard error: 4.699 on 8 degrees of freedom
```

```
Multiple R-squared: 0.9643, Adjusted R-squared: 0.9509
```

```
F-statistic: 71.95 on 3 and 8 DF,  p-value: 3.956e-06
```

result: the more complex model, in which different species react differently to low food level, fits significantly better.



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But can we really assume normal distribution on numbers like 5, 8, 9...?

result: the more complex model, in which different species react differently to low food level, fits significantly better.

But can we really assume normal distribution on numbers like 5, 8, 9...?

We will come back to this in the Lecture about GLMs.

# Contents

Regression toward the mean

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- root of numbers of inhabitants and deaths

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- Example: Success of different therapies

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Cross validation and AIC

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```
prederrorHL <- numeric()
for (i in 1:46) {
  selection <- rep(TRUE,46)
  selection[i] <- FALSE
  modHL.R <- lm(WingL~N.UBkL+BeakH,data=finchdata,
                subset=selection)
  prederrorHL[i]=WingL[i]-predict(modHL.R,finchdata[i,])
}
```



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