

Multivariate Statistics in Ecology and Quantitative Genetics

Linear Regression and Linear Models

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http://evol.bio.lmu.de/_statgen

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Contents

Univariate linear regression

t-test for linear regression

Multivariate Regression

Example: species richness on sandy beaches

Example: Success of different therapies

Cross validation and AIC

Example: Beak sizes and winglengths in Darwin finches

Example: Overfitting

Example: Daphnia



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

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- ▶ Developed telemetric system for measuring heart beats of flying birds



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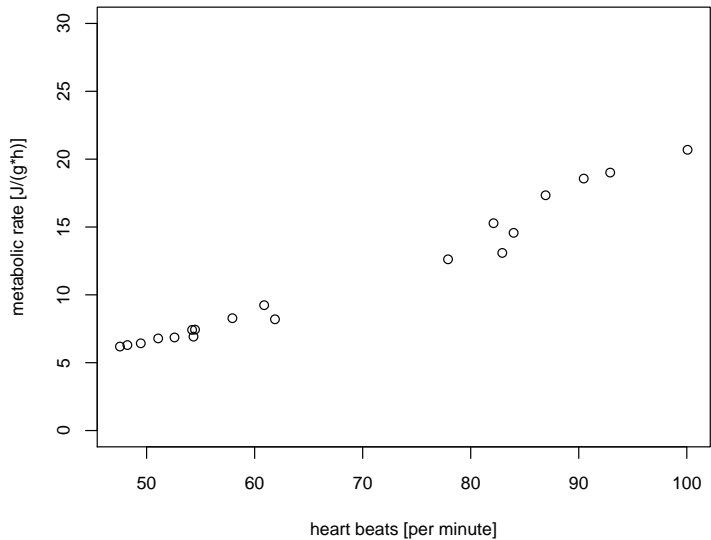
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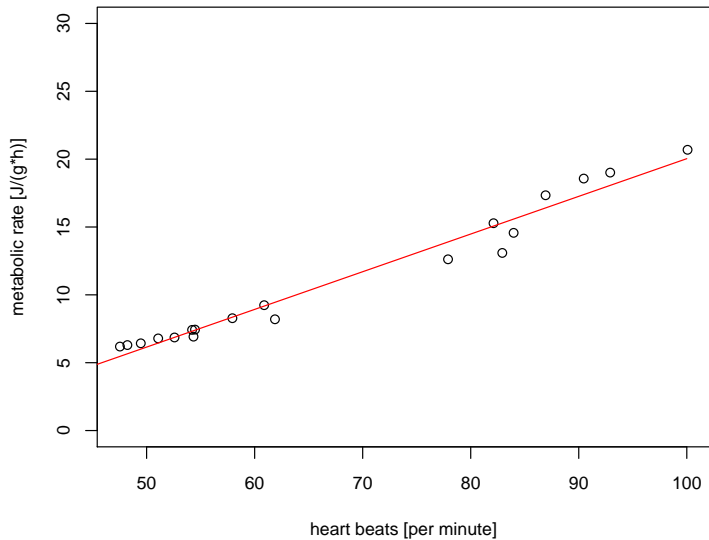


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- ▶ Data from Goethe-University, Group of Prof. Prinzinger
- ▶ Developed telemetric system for measuring heart beats of flying birds
- ▶ Important for ecological questions: metabolic rate.
- ▶ metabolic rate can only be measured in the lab
- ▶ can 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
.
.
.

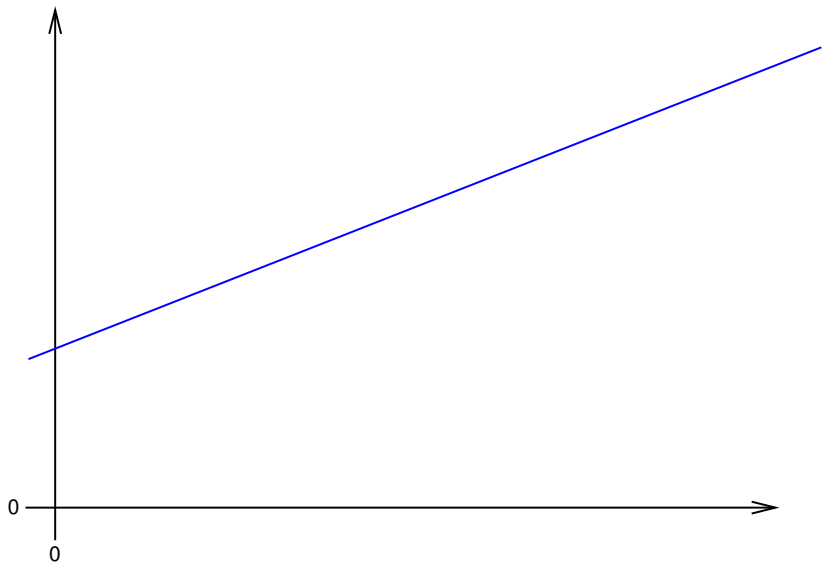
(14 different days)

```

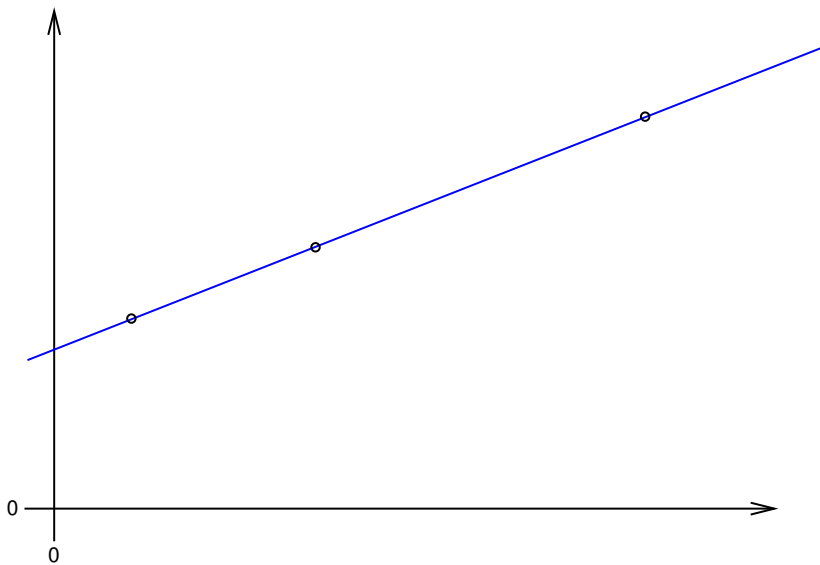
> model <- lm(metabol~heartbpm,data=vulture,
              subset=day=="17.05.")
> summary(model)
Call:
lm(formula = metabol ~ heartbpm, data = vulture, subset = day
    "17.05.")
Residuals:
    Min       1Q   Median       3Q      Max
-2.2026 -0.2555  0.1005  0.6393  1.1834
Coefficients:
                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

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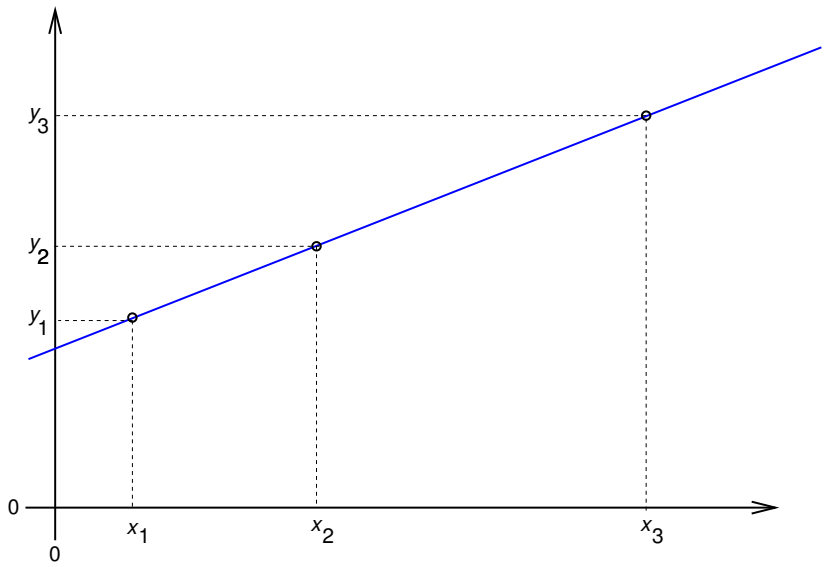
Univariate linear regression



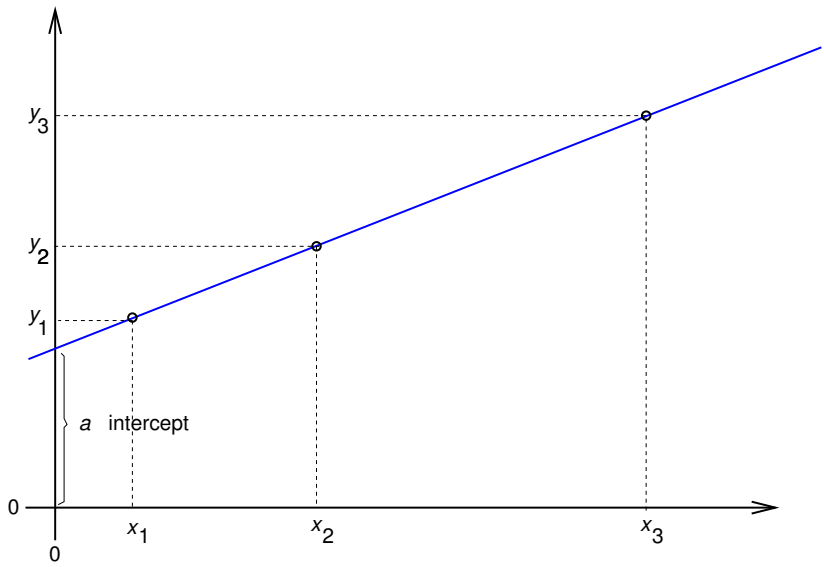
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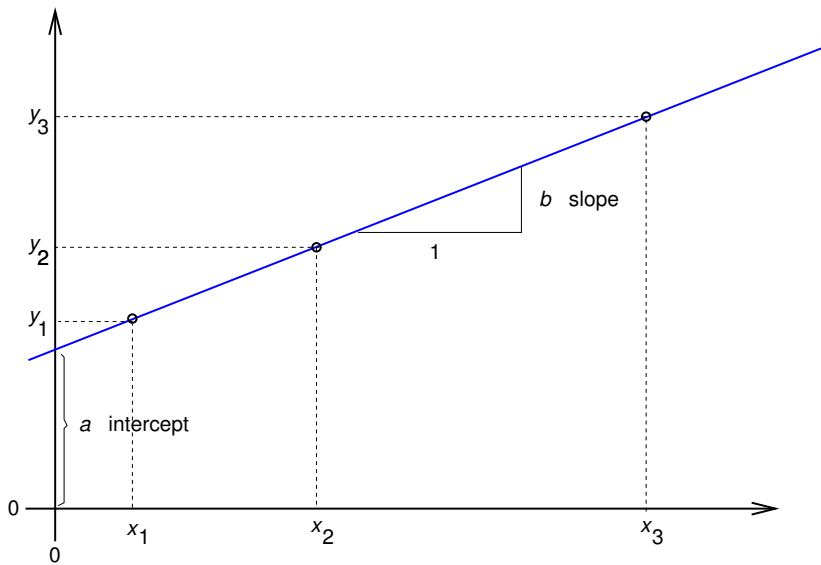
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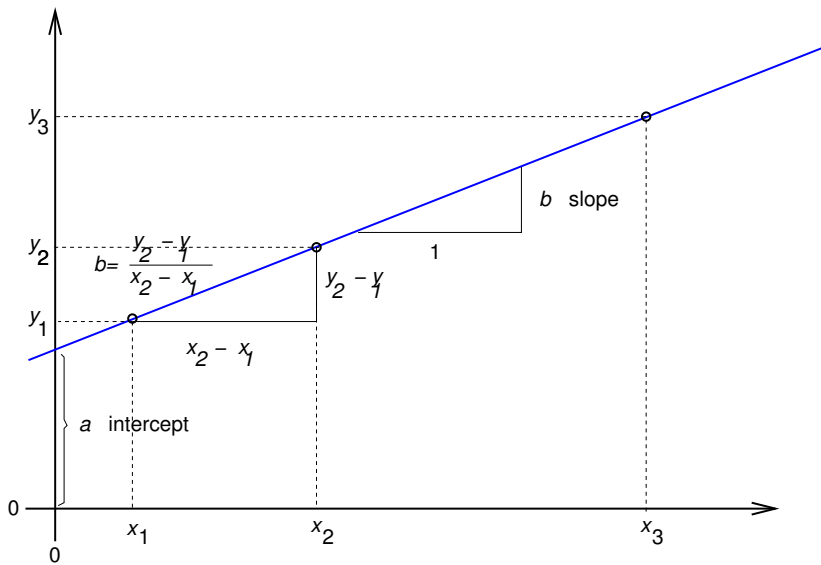
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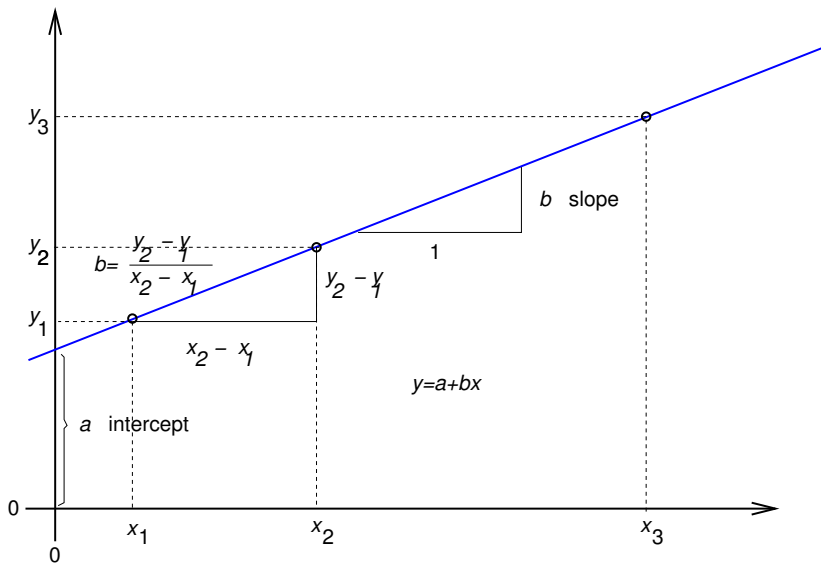
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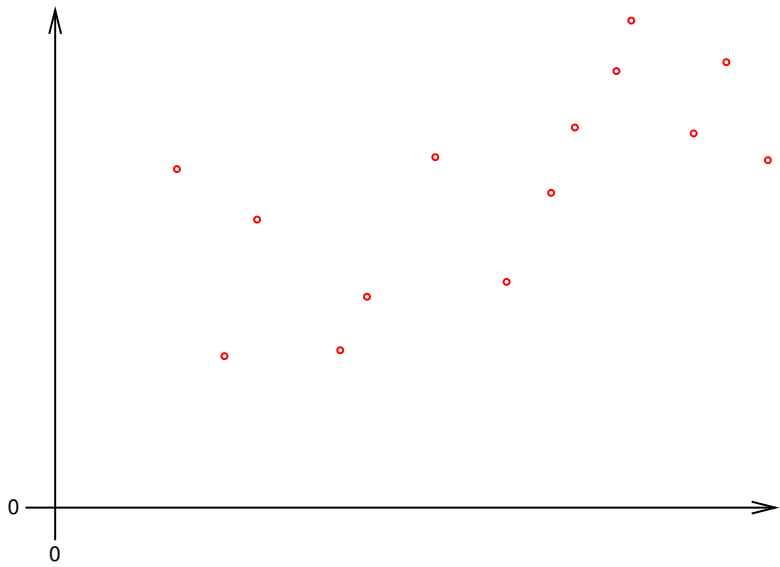
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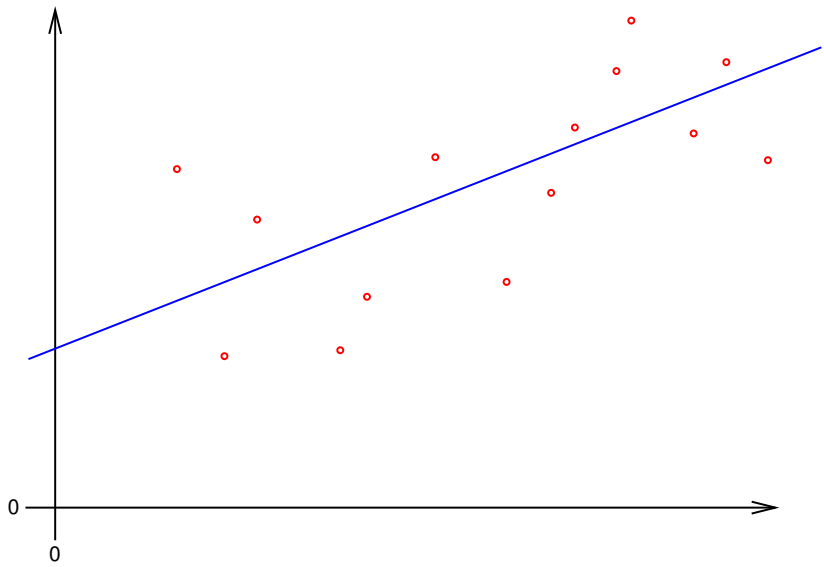
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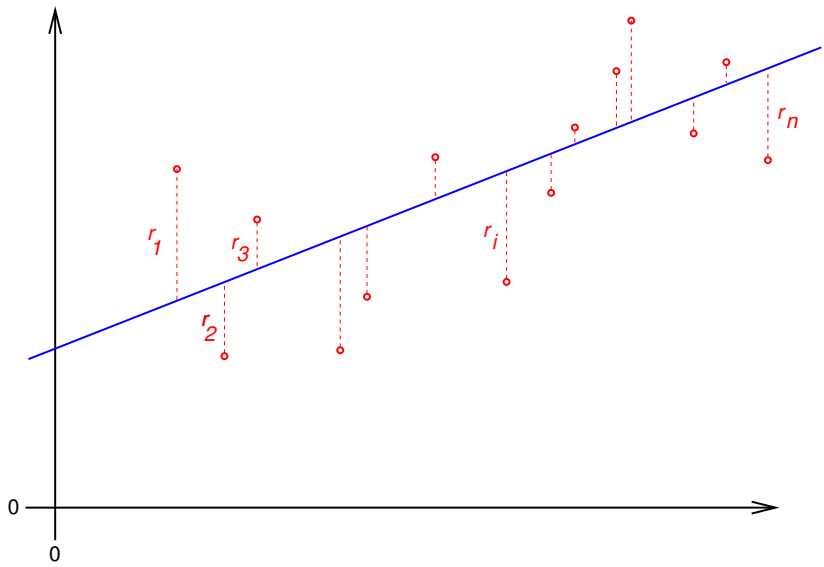
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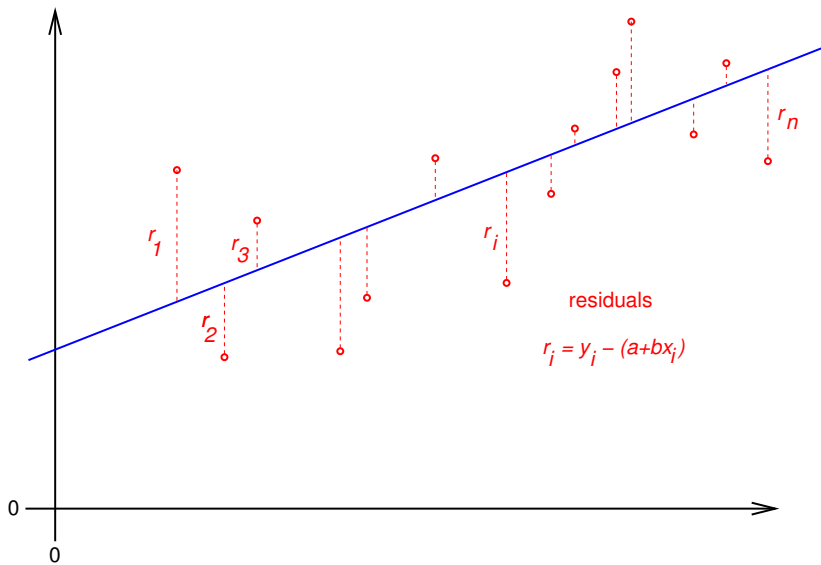
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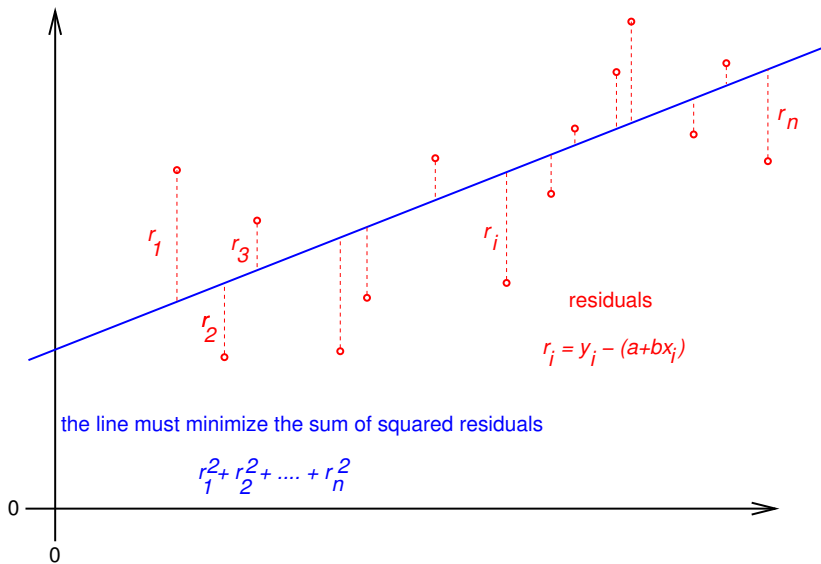


Univariate linear regression



Univariate linear regression





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 ε_i are independent and normally distributed with the same variance σ^2 .

given data:

Y	X
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, σ^2 such that

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

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

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$$\vdots \quad \vdots$$

$$y_n = a + b \cdot x_n + \varepsilon_n$$

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$$\begin{aligned}y_1 &= a + b \cdot x_1 + \varepsilon_1 \\y_2 &= a + b \cdot x_2 + \varepsilon_2 \\y_3 &= a + b \cdot x_3 + \varepsilon_3 \\&\vdots \\&\vdots \\y_n &= a + b \cdot x_n + \varepsilon_n\end{aligned}$$

$\varepsilon_1, \varepsilon_2, \dots, \varepsilon_n$ 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, σ^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 $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$.

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(14 different days)

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> model <- lm(metabol~heartbpm,data=vulture,
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```
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Residuals:

Min	1Q	Median	3Q	Max
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Coefficients:

	Estimate	Std. Error	t value	Pr(> t)
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Example: Success of different therapies

Cross validation and AIC

Example: Beak sizes and winglengths in Darwin finches

Example: Overfitting

Example: Daphnia

t-test for \hat{b}

Estimate σ^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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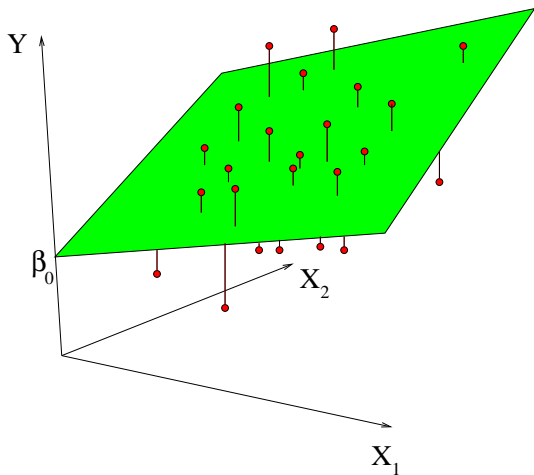
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Observations:

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

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

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

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

Multivariate Regression

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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 σ^2 .

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Example: Daphnia

- ▶ 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

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- ▶ 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.

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.

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.

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.

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.

- ▶ Obviously, in weeks 2 and 3 significantly less species were found than in week 1, which is our reference point here.
- ▶ The estimated `Intercept` is thus the expected species richness in week 1 in a plot where all other parameters take the value 0.

- ▶ Obviously, in weeks 2 and 3 significantly less species were found than in week 1, which is our reference point here.
- ▶ 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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We saw before that weeks 2 and 3 are significantly different from week 1.

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

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

We saw before that weeks 2 and 3 are significantly different from week 1. However, the p value refers to the situation of single testing.

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.

Bonferroni correction

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

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

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

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

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

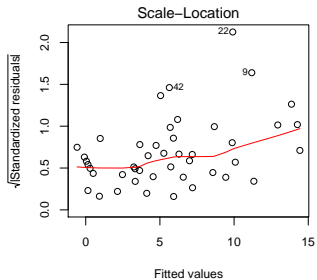
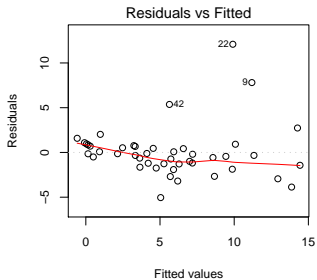
	Res.Df	RSS	Df	Sum of Sq	F	Pr(>F)
1	40	531.17				
2	37	353.66	3	177.51	6.1902	0.00162 **

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

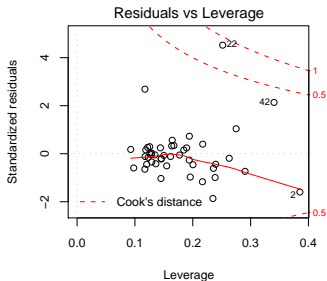
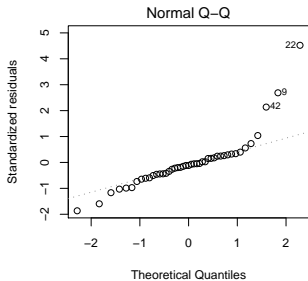
We reject the null hypothesis that the weeks have no effect with a p -value of 0.00162.

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.

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

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	***
factor(week)3	-5.719055	1.827616	-3.129	0.0034	**
factor(week)4	-1.481816	2.720089	-0.545	0.5891	

```
---
```

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

Contents

Univariate linear regression

t-test for linear regression

Multivariate Regression

Example: species richness on sandy beaches

Example: Success of different therapies

Cross validation and AIC

Example: Beak sizes and winglengths in Darwin finches

Example: Overfitting

Example: Daphnia

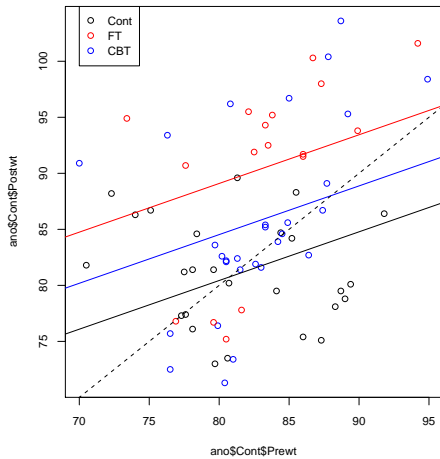
For young anorexia patients the effect of family therapy (FT) and cognitive behavioral therapy (CBT) is compared to a control group (Cont) by comparing the weight before (Prewt) and after (Postwt) the treatment (Treat).



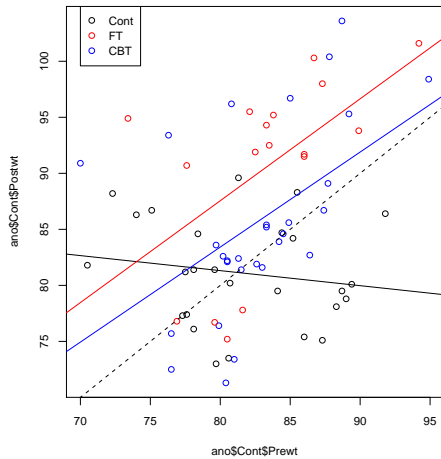
Hand, D. J., Daly, F., McConway, K., Lunn, D. and Ostrowski, E. eds (1993) *A Handbook of Small Data Sets*. Chapman & Hall

- 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 Preweight.
- 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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Multivariate Regression

Example: species richness on sandy beaches

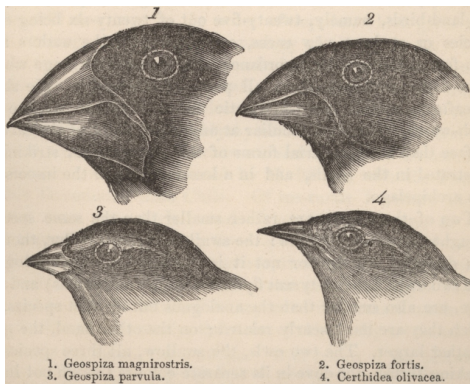
Example: Success of different therapies

Cross validation and AIC

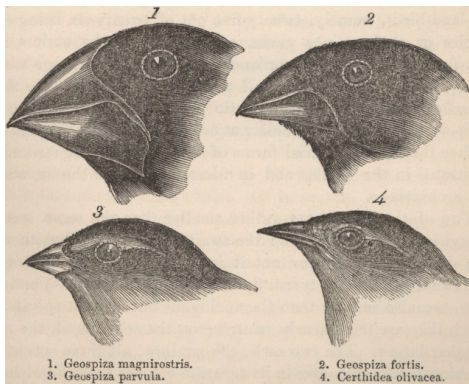
Example: Beak sizes and winglengths in Darwin finches

Example: Overfitting

Example: Daphnia

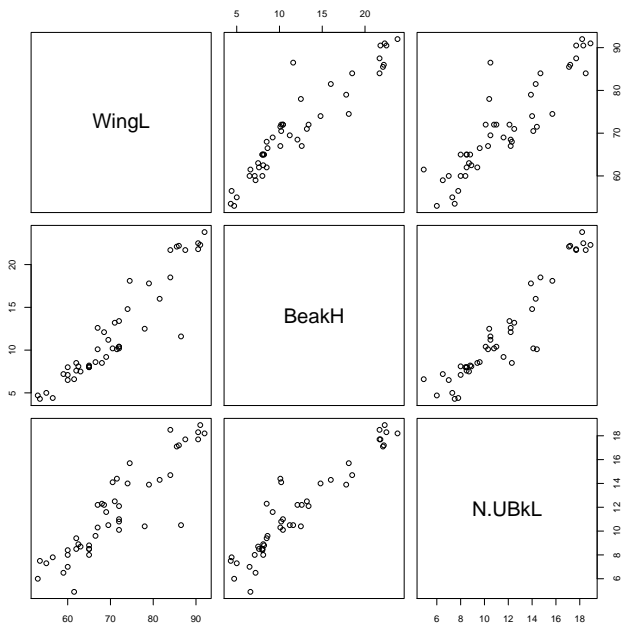


You find a beak of a Darwin finch. The beak is 14 mm long and 10 mm high. How accurately can you predict the winglength of the bird?



You find a beak of a Darwin finch. The beak is 14 mm long and 10 mm high. How accurately can you predict the winglength of the bird?

Your “training data” are the winglengths (WingL), beak heights (BeakH) and beak lengths (N.UBkL) of 46 Darwin finches.



```
> modH <- lm(WingL~BeakH)
> summary(modH)
```

```
Call:
lm(formula = WingL ~ BeakH)
```

```
Residuals:
```

```
      Min       1Q   Median       3Q      Max
-7.1882 -2.5327 -0.2796  1.8325 16.2702
```

```
Coefficients:
```

```
              Estimate Std. Error t value Pr(>|t|)
(Intercept)  49.78083    1.33103   37.40  <2e-16 ***
BeakH         1.76284    0.09961   17.70  <2e-16 ***
```

```
---
```

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

```
Residual standard error: 3.868 on 44 degrees of freedom
```

```
Multiple R-squared:  0.8768, Adjusted R-squared:  0.874
```

```
F-statistic: 313.2 on 1 and 44 DF,  p-value: < 2.2e-16
```

```
> predict(modH,newdata=data.frame(BeakH=10))
```

```
      1
67.40924
```

```
> modL <- lm(WingL~N.UBkL)
> summary(modL)
```

```
Call:
lm(formula = WingL ~ N.UBkL)
```

```
Residuals:
```

Min	1Q	Median	3Q	Max
-7.1321	-3.3974	0.4737	2.2966	18.2299

```
Coefficients:
```

	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	41.5371	2.2884	18.15	<2e-16 ***
N.UBkL	2.5460	0.1875	13.58	<2e-16 ***

```
---
```

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

```
Residual standard error: 4.838 on 44 degrees of freedom
```

```
Multiple R-squared: 0.8074, Adjusted R-squared: 0.803
```

```
F-statistic: 184.4 on 1 and 44 DF, p-value: < 2.2e-16
```

```
> predict(modL,newdata=data.frame(N.UBkL=14))
```

```
1
77.18117
```

```
> modHL <- lm(WingL~BeakH+N.UBkL)
> summary(modHL)
```

```
Call:
lm(formula = WingL ~ BeakH + N.UBkL)
```

```
Residuals:
```

```
      Min       1Q   Median       3Q      Max
-7.3185 -2.5022 -0.2752  1.5352 16.5893
```

```
Coefficients:
```

	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	48.1740	2.2572	21.343	< 2e-16 ***
BeakH	1.5133	0.2999	5.047	8.69e-06 ***
N.UBkL	0.3984	0.4513	0.883	0.382

```
---
```

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

```
Residual standard error: 3.878 on 43 degrees of freedom
```

```
Multiple R-squared:  0.879, Adjusted R-squared:  0.8734
```

```
F-statistic: 156.2 on 2 and 43 DF,  p-value: < 2.2e-16
```

```
> predict(modHL,newdata=data.frame(BeakH=10,N.UBkL=14))
```

```
      1
68.88373
```

Which of the three predictions 67.4mm, 77.2mm und 68.9mm for the winglength is most reliable?

Which of the three predictions 67.4mm, 77.2mm und 68.9mm for the winglength is most reliable?

In the model modHL (with beak length and height) the influence of beak length is not significant.

Which of the three predictions 67.4mm, 77.2mm und 68.9mm for the winglength is most reliable?

In the model modHL (with beak length and height) the influence of beak length is not significant.

We can not draw conclusion from non-significance. Beak length could still improve the prediction.

Which of the three predictions 67.4mm, 77.2mm und 68.9mm for the winglength is most reliable?

In the model modHL (with beak length and height) the influence of beak length is not significant.

We can not draw conclusion from non-significance. Beak length could still improve the prediction.

Is it always good to use as much data as possible?

Which of the three predictions 67.4mm, 77.2mm und 68.9mm for the winglength is most reliable?

In the model modHL (with beak length and height) the influence of beak length is not significant.

We can not draw conclusion from non-significance. Beak length could still improve the prediction.

Is it always good to use as much data as possible?

This could lead to “overfitting”: If too many parameters are available, the model will learn all the little details of the data including random fluctuations. It will learn just memorize the training data. This may corrupt the model’s predictions for new data.

We could judge the models by the standard deviation of the ε_i , which we estimate by the standard deviation of the residuals r_i .

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We must account for the different number d of model parameters, because we lose one degree of freedom for each estimated parameter:

$$\hat{\sigma}_\varepsilon = \sqrt{\frac{1}{n-d} \sum_i r_i^2} = \sigma_r \cdot \sqrt{\frac{n-1}{n-d}}.$$

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These values are reported in R by the command “summary”:

modH:

Residual standard error: 3.868 on 44 degrees of freedom

modL:

Residual standard error: 4.838 on 44 degrees of freedom

modHL:

Residual standard error: 3.878 on 43 degrees of freedom

Another possibility to judge the prediction error of a model is *cross validation* (aka *Jackknife*).

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The idea is: Remove one of the 46 birds from the dataset and fit the model to the other 45. How well can the model predict the winglength of the omitted bird?

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Repeat this for all 46 birds.

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Repeat this for all 46 birds.

We have to decide how we measure the error. How to judge a model with many medium errors compared to a model with rare large errors? We use (the square root of) the sum of squared errors.

```
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,])
}
```

	Height	Length	Height and Length
$\sigma(\text{Residuals})$	3.83	4.78	3.79

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Akaike's Information Criterion:

$$\text{AIC} = -2 \cdot \log L + 2 \cdot (\text{Number of Parameters})$$

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$$\text{AIC} = -2 \cdot \log L + 2 \cdot (\text{Number of Parameters})$$

Bayesian Information Criterion:

$$\text{BIC} = -2 \cdot \log L + \log(n) \cdot (\text{Number of Parameters})$$

For $n \geq 8$ holds $\log(n) > 2$ and BIC penalizes every additional parameter harder than AIC. (As always, \log is the natural logarithm.)

Low values of AIC and BIC favor the model.

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AIC is based on the idea to approximate the prediction error (which is exact under certain conditions).

BIC approximates (up to a constant) the log of the posterior probability of the model, where all models are a priori assumed to be equally probable.

	height	length	height and length
$\sigma(\text{Residuals})$	3.83	4.78	3.79
$d = (\text{Number of parameters})$	2	2	3
$\sigma(\text{Residuals}) \cdot \sqrt{\frac{n-1}{n-d}}$	3.87	4.84	3.88
cross validation.	26.56	33.34	26.68
AIC	259.0	279.5	260.1
BIC	264.4	285.0	267.4

It seems best to use only the beak height.

Problem with extensive model selection

If you have optimized the model e.g. by AIC and then compute p -values with the same data, you find too much significance.

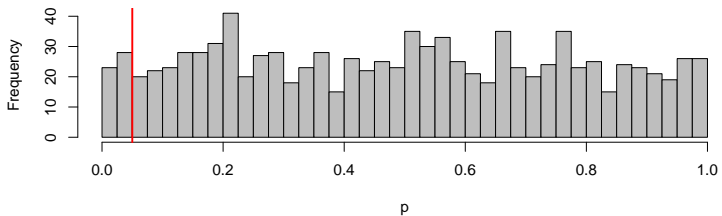
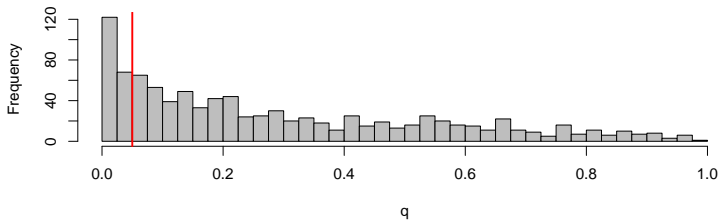
Problem with extensive model selection

If you have optimized the model e.g. by AIC and then compute p -values with the same data, you find too much significance. We explore this with a little simulation:

```
A <- as.factor(rep(c("a","b","c"),c(40,40,40)))
B <- as.factor(rep(rep(c("w","x","y","z"),c(10,10,10,10)),3))
C <- as.factor(rep(c("p","q","r"),40))
D <- as.factor(rep(rep(c("m","n"),c(5,5)),12))
X <- rnorm(120,10,2)
```

```
library(MASS)
```

```
p <- numeric()
q <- numeric()
for(i in 1:1000) {
  X <- rnorm(120,10,2)
  p[i] <- anova(lm(X~1),lm(X~A*B*C*D))$"Pr(>F)" [[2]]
  q[i] <- anova(lm(X~1),stepAIC(lm(X~A*B*C*D))$"Pr(>F)" [[2]]
}
```

Histogram of p Histogram of q 

Save model selection and checking if you have lots of data

1. Divide the data randomly into 3 subsets A, B, C, where A may contain half of the data, and B and C a quarter each.
2. Fit each candidate model to the data subset A.
3. Assess the accuracy of these fitted models with data subset B. Let M be the best model in this contest.
4. Assess the accuracy of M again and also its p -values, this time with dataset C.

Graphical methods are also very important in model fitting, especially applied to residuals. Plot residuals against variables. If this uncovers dependencies, they should be added to the model.

Contents

Univariate linear regression

t-test for linear regression

Multivariate Regression

Example: species richness on sandy beaches

Example: Success of different therapies

Cross validation and AIC

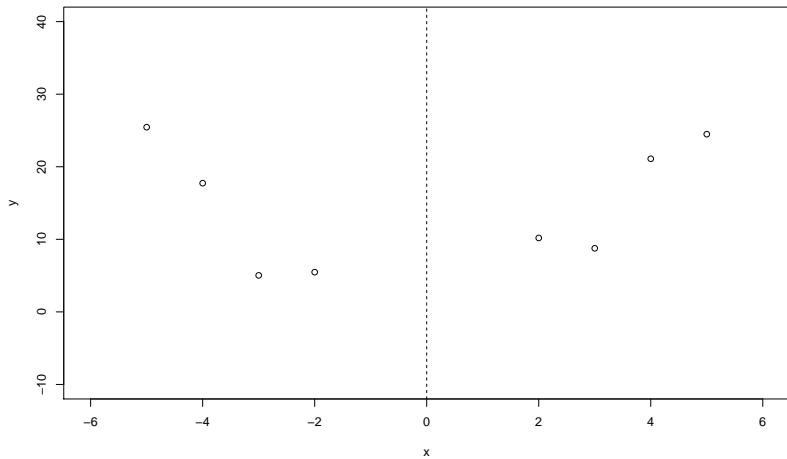
Example: Beak sizes and winglengths in Darwin finches

Example: Overfitting

Example: Daphnia

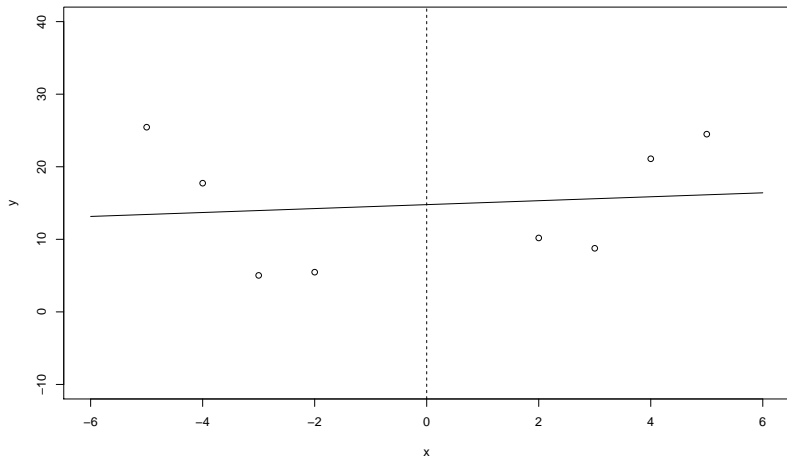
Overfitting

What is the value of y for $x=0$?



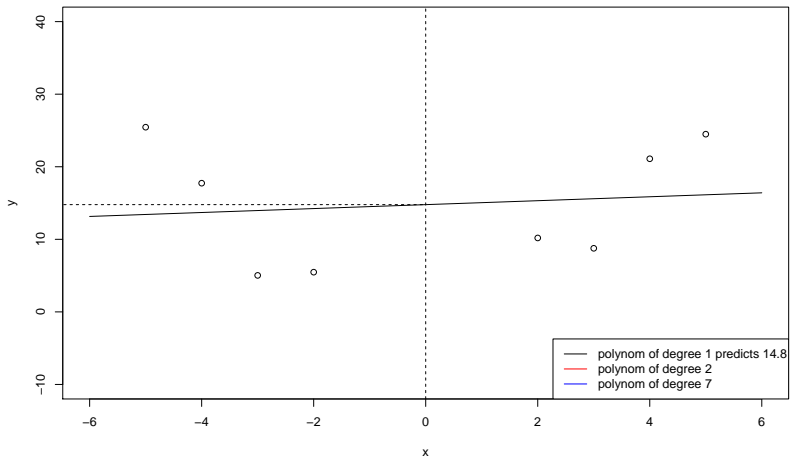
Overfitting

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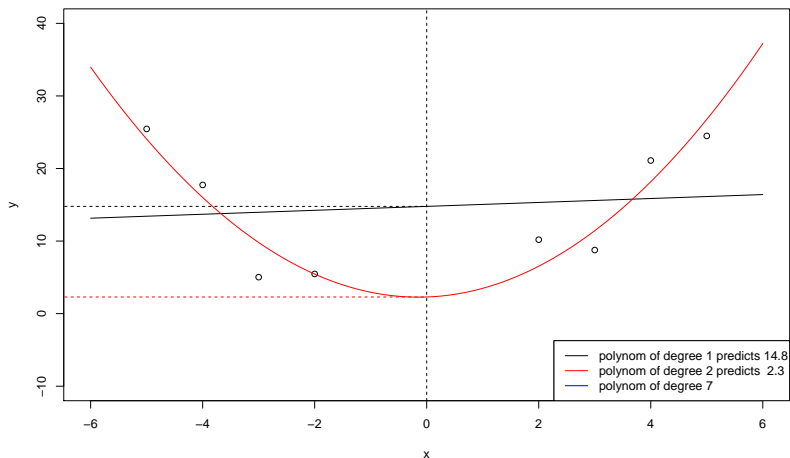
Overfitting

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Overfitting

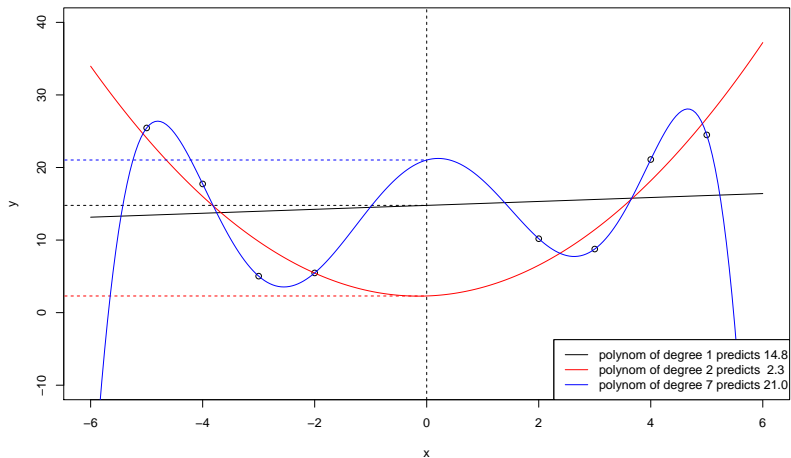
What is the value of y for $x=0$?



$\text{lm}(y \sim \text{poly}(x, 2))$ is the same as $\text{lm}(y \sim x + I(x^2))$

Overfitting

What is the value of y for $x=0$?



$\ln(y \sim \text{poly}(x, 7))$

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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
```

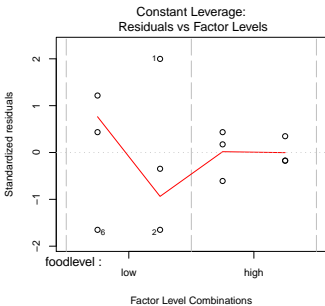
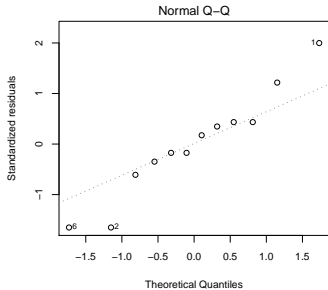
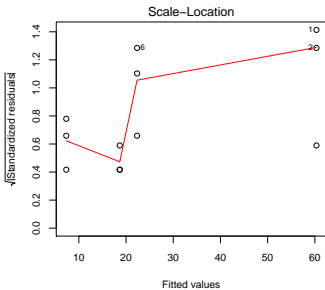
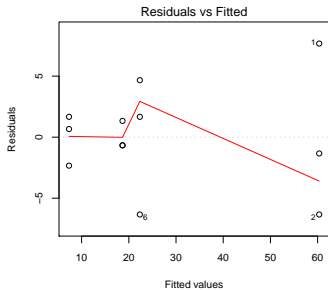
```
Multiple R-squared: 0.9643, Adjusted R-squared: 0.9509
```

```
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 does it fit well enough...?



```
> mod3 <- lm(log(counts)~foodlevel+species,data=daph)
> mod4 <- lm(log(counts)~foodlevel*species,data=daph)
> anova(mod3,mod4)
```

Analysis of Variance Table

Model 1: $\log(\text{counts}) \sim \text{foodlevel} + \text{species}$

Model 2: $\log(\text{counts}) \sim \text{foodlevel} * \text{species}$

	Res.Df	RSS	Df	Sum of Sq	F	Pr(>F)
1	9	0.38041				
2	8	0.37856	1	0.0018545	0.0392	0.848

```
> summary(mod3)
```

```
Call:
```

```
lm(formula = log(counts) ~ foodlevel + species, data = daph)
```

```
Residuals:
```

	Min	1Q	Median	3Q	Max
	-0.34017	-0.05915	0.02622	0.13153	0.24762

```
Coefficients:
```

	Estimate	Std. Error	t value	Pr(> t)	
(Intercept)	3.0946	0.1028	30.104	2.41e-10	***
foodlevellow	-1.1450	0.1187	-9.646	4.83e-06	***
speciesmagna	0.9883	0.1187	8.326	1.61e-05	***

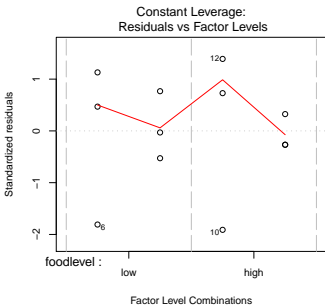
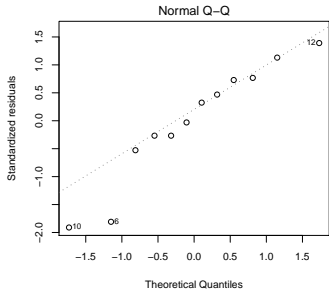
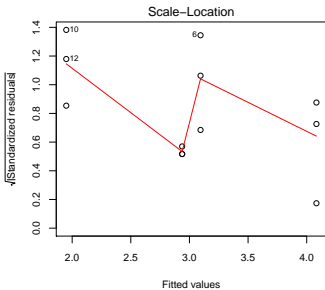
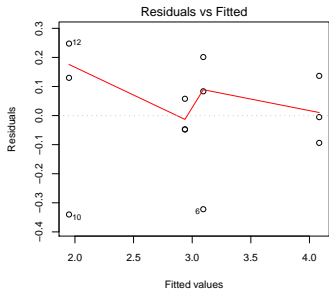
```
---
```

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

```
Residual standard error: 0.2056 on 9 degrees of freedom
```

```
Multiple R-squared: 0.9475, Adjusted R-squared: 0.9358
```

```
F-statistic: 81.19 on 2 and 9 DF,  p-value: 1.743e-06
```



The qqplot looks better now but not really good.

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The reason is perhaps that the values of the target variable `counts` were small integers such that the normal distribution assumption is dubious.

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Instead of the normal linear model we can fit a log transformed generalized linear model of type Poisson. We will see this in a few days.

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Instead of the normal linear model we can fit a log transformed generalized linear model of type Poisson. We will see this in a few days.

For now we only compare the models with normality assumptions.

```
> AIC(mod1,mod2,mod3,mod4)
      df      AIC
mod1  4 91.0188246
mod2  5 76.3268216
mod3  4  0.6376449
mod4  5  2.5790019
```

The log-linear models clearly have better AIC values than the linear models with untransformed data. But one should not compare AIC values between models with different (or differently scaled) target variable.

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The log-linear models clearly have better AIC values than the linear models with untransformed data. But one should not compare AIC values between models with different (or differently scaled) target variable.

The interaction in model mod4 is not only non-significant, the model mod3 without interaction also has the better AIC values.

So we favor mod3:

$$\log(\text{counts}) = 3.09 - 1.14 \cdot I_{\text{low food}} + 0.99 \cdot I_{\text{magna}} + \varepsilon$$

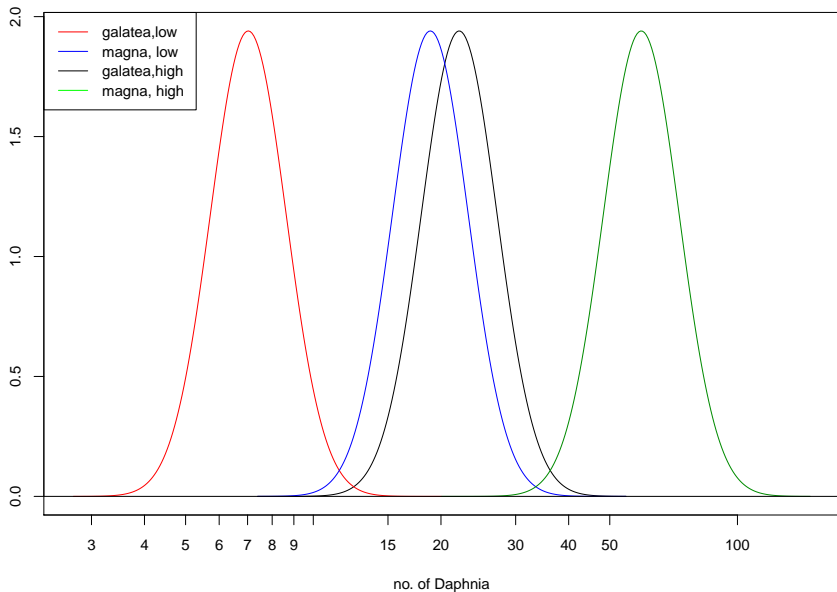
So we favor mod3:

$$\log(\text{counts}) = 3.09 - 1.14 \cdot I_{\text{low food}} + 0.99 \cdot I_{\text{magna}} + \varepsilon$$

By applying the e function we obtain:

$$\text{counts} = 21.98 \cdot 0.32^{I_{\text{low food}}} \cdot 2.69^{I_{\text{magna}}} \cdot e^{\varepsilon}$$

prediction of log-linear model



But is it reasonable at all to assume normal distribution when the data are counts $0, 1, 2, \dots$?

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We will come back to this dataset when we discuss GLMs.