Kurs Bio144: Datenanalyse in der Biologie

Lecture 3: Simple linear regression

Stefanie Muff (Lecture) & Owen L.Petchey (Practical)

University of Zurich

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Overview

- Introduction of the linear regression model
- Parameter estimation
- Simple model checking
- Goodness of the model: Correlation and R^2
- Tests and confidence intervals
- Confidence and prediction ranges

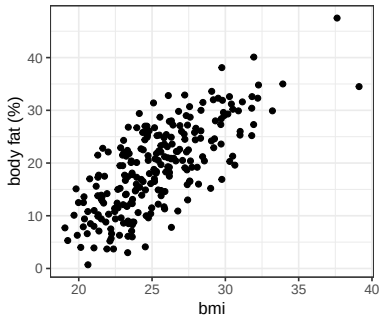
Course material covered today

The lecture material of today is based on the following literature:

- Chapter 2 of *Lineare Regression*, p.7-20 (Stahel script)

The body fat example

Remember: Aim is to find prognostic factors for body fat, without actually measuring it.
Even simpler question: How good is BMI as a predictor for body fat?



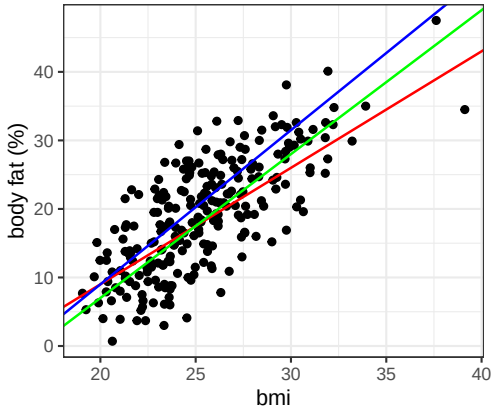
Linear relationship

- The most simple relationship between an *explanatory variable* (X) and a *target/outcome variable* (Y) is a linear relationship. All points (x_i, y_i), $i = 1, \ldots, n$, on a straight line follow the equation

$$y_i = \alpha + \beta x_i \ .$$

- Here, α is the axis intercept and β the slope of the line. β is also denoted as the regression coefficient of X.
- If $\alpha = 0$ the line goes through the origin $(x, y) = (0, 0)$.
- Interpretation of linear dependency: proportional increase in y with increase (decrease) in x.

But which is the “true” or “best” line?



Task: Estimate the regression parameters α and β (by “eye”) and write them down.

It is obvious that

- the linear relationship does not describe the data perfectly
- another realization of the data (other 243 males) would lead to a slightly different picture.

$\Rightarrow$ We need a **model** that describes the relationship between BMI and bodyfat.

The simple linear regression model

In the linear regression model the dependent variable Y is related to the independent variable x as

$$Y = \alpha + \beta x + \epsilon \,, \qquad \epsilon \sim N(0, \sigma^2)$$

In this formulation Y is a random variable $Y \sim N(\alpha + \beta x, \sigma^2)$ where

$$Y \quad = \quad \underbrace{\text{expected value}}_{E(Y)=\alpha+\beta x} \quad + \quad \underbrace{\text{random error}}_{\epsilon} \,.$$

Note:

- The model for Y given x has three parameters: α, β and σ^2 .
- x is the independent / explanatory / regressor variable.
- Y is the dependent / outcome / response variable.

Note

- The linear model propagates the most simple relationship between two variables. When using it, please always think if such a relationship is meaningful/reasonable/plausible.
- Always look at the data before you start with model fitting.

Visualization of the regression assumptions

The assumptions about the linear regression model lie in the error term

$$\epsilon \sim N(0, \sigma^2) \ .$$

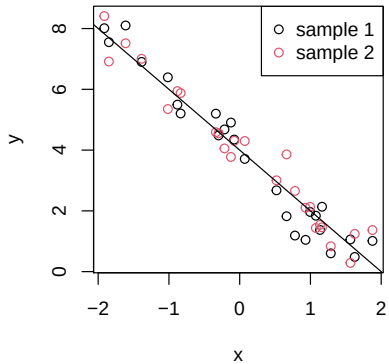
Note: The true regression line goes through $E(Y)$.

Insights from data simulation

(Simulation are *always* a great way to understand statistics!!)

Generate an independent (explanatory) variable **x** and **two** samples of a dependent variable **y** assuming that

$$y_i = 4 - 2x_i + \epsilon_i \ , \quad \epsilon_i \sim N(0, 0.5^2) \ .$$



→ Random variation is always present. This leads us to the next question.

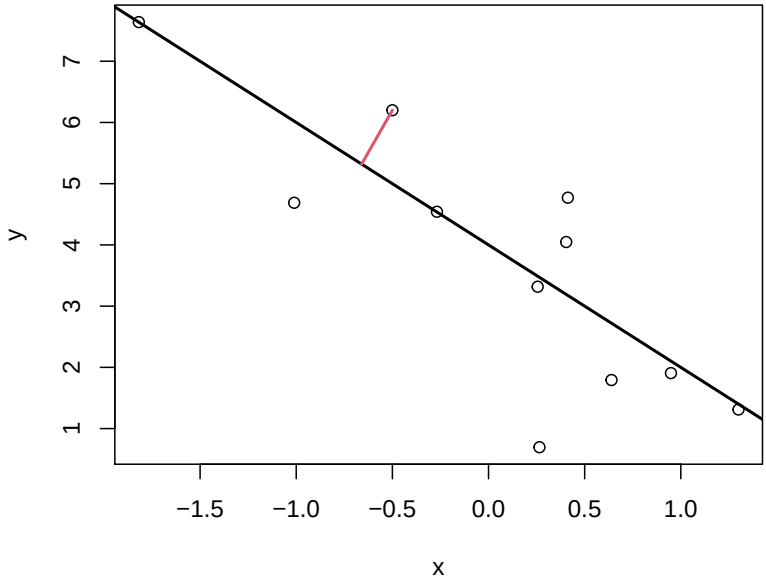
Parameter estimation

In a regression analysis, the task is to estimate the regression coefficients α, β and the residual variance σ^2 for a given set of (x, y) data.

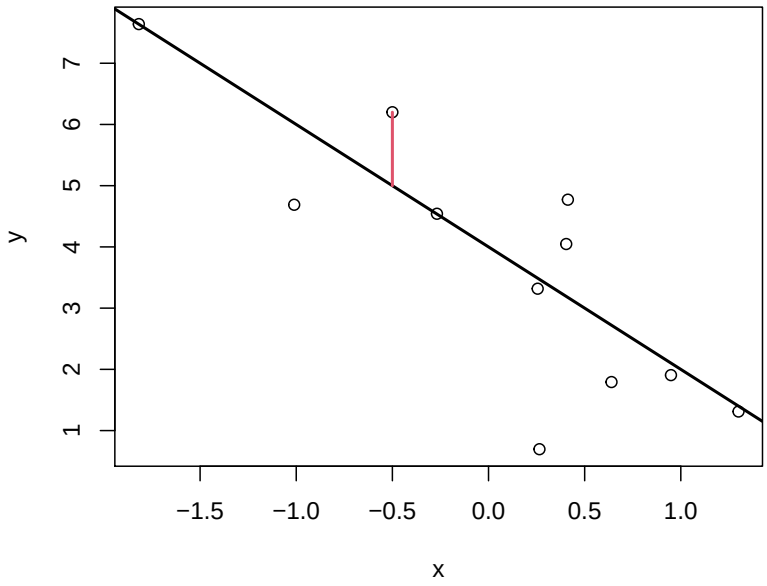
- **Problem:** For more than two points (x_i, y_i), $i = 1, \ldots, n$, there is generally no perfectly fitting line.
- **Aim:** We want to find the parameters (a, b) of the best fitting line $Y = a + bx$.
- **Idea:** Minimize the deviations between the data points (x_i, y_i) and the regression line.

But how?

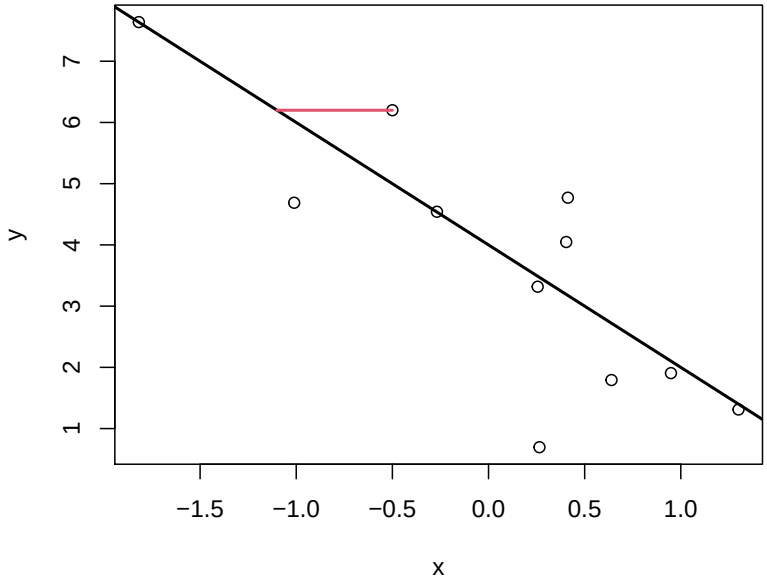
Should we minimize these distances. . .



Or these?



Or maybe even these?



Least squares

For multiple reasons (theoretical aspects and mathematical convenience), the parameters are estimated using the least squares approach. In this, yet something else is minimized:

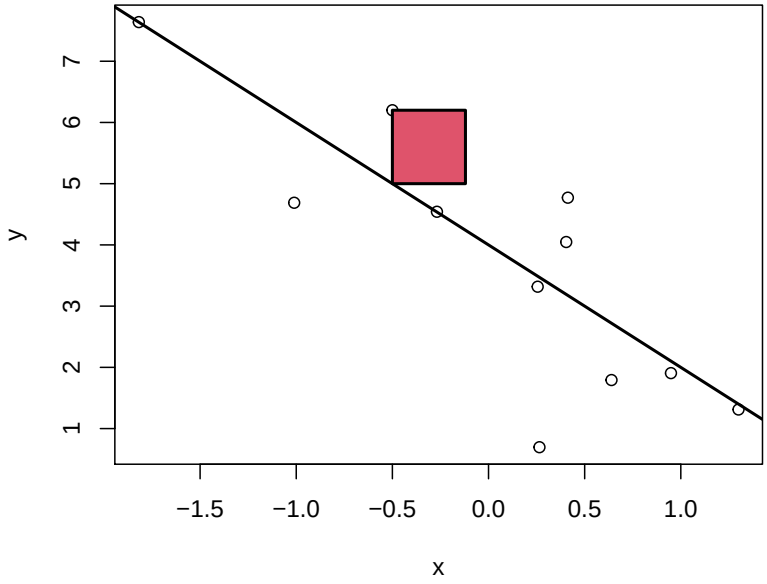
The parameters α and β are estimated such that the sum of squared vertical distances (sum of squared residuals)

$$SSE = \sum_{i=1}^{n} e_i^2 \,, \qquad \text{where} \quad e_i = y_i - \underbrace{(a + bx_i)}_{=\hat{y}_i}$$

is being minimized.

Note: $\hat{y}_i = a + bx_i$ are the predicted values.

So we minimize the sum of these areas!



Least squares estimates

For a given sample $(x_i, y_i), i = 1, .., n$, with mean values $\overline{x}$ and $\overline{y}$, the least squares estimates $\hat{\alpha}$ and $\hat{\beta}$ are computed as

$$\begin{aligned} \hat{\beta} &= \frac{\sum_{i=1}^{n}(y_i - \overline{y})(x_i - \overline{x})}{\sum_{i=1}^{n}(x_i - \overline{x})^2} = \frac{cov(x, y)}{var(x)} , \\ \hat{\alpha} &= \overline{y} - \hat{\beta}\overline{x} . \end{aligned}$$

Moreover,

$$\hat{\sigma}^2 = \frac{1}{n-2}\sum_{i=1}^{n} e_i^2 \quad \text{with residuals } e_i = y_i - (\hat{\alpha} + \hat{\beta}x_i)$$

is an unbiased estimate of the residual variance σ^2.

(The derivation of the parameters can be looked up in the Stahel script 2.A b. Idea: Minimization through derivating equations and setting them =0.)

Do-it-yourself “by hand”

Go to the Shiny gallery and try to “estimate’ ’ the correct parameters.

You can do this here:

https://gallery.shinyapps.io/simple_regression/

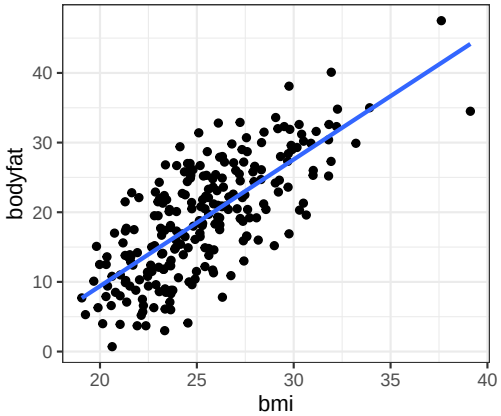
Estimation using R

Let's estimate the regression parameters from the bodyfat example

```
r.bodyfat <- lm(bodyfat ~ bmi,d.bodyfat)
summary(r.bodyfat)
```

```
##
## Call:
## lm(formula = bodyfat ~ bmi, data = d.bodyfat)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -13.5485  -3.5583   0.0785   4.0384  12.7330
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept) -26.9844     2.7689  -9.746   <2e-16 ***
## bmi           1.8188     0.1083  16.788   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 5.573 on 241 degrees of freedom
## Multiple R-squared:  0.539,  Adjusted R-squared:  0.5371
## F-statistic: 281.8 on 1 and 241 DF,  p-value: < 2.2e-16
```

The resulting line can be added to the scatterplot:



Interpretation: for an increase in the BMI by one index point, we roughly expect a 1.82% percentage increase in bodyfat.

Uncertainty in the estimates $\hat{\alpha}$ and $\hat{\beta}$

Important: $\hat{\alpha}$ and $\hat{\beta}$ are themselves random variables and as such contain uncertainty!

Let us look again at the regression output, this time only for the coefficients. The second column shows the standard error of the estimate:

```
summary(r.bodyfat)$coef
```

```
##               Estimate Std. Error   t value     Pr(>|t|)
## (Intercept) -26.984368  2.7689004 -9.745518 3.921511e-19
## bmi           1.818778  0.1083411 16.787522 2.063854e-42
```

$\rightarrow$ The logical next question is: what is the distribution of the estimates?

Distribution of the estimators for $\hat{\alpha}$ and $\hat{\beta}$

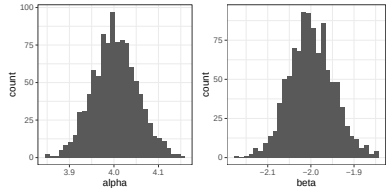
To obtain an idea, we generate data points according to model

$$y_i = 4 - 2x_i + \epsilon_i \ , \quad \epsilon_i \sim N(0, 0.5^2).$$

In each round, we estimate the parameters and store them:

```
niter <- 1000
pars <- matrix(NA,nrow=niter,ncol=2)
for (ii in 1:niter){
  x <- rnorm(100)
  y <- 4 - 2*x + rnorm(100,0,sd=0.5)
  pars[ii,] <- lm(y~x)$coef
}
```

Doing it 1000 times, we obtain the following distributions for $\hat{\alpha}$ and $\hat{\beta}$:



This looks suspiciously normal!

In fact, from theory it is known that

$$\hat{\beta} \sim N(\beta, \sigma^{(\beta)2}) \qquad \text{and} \qquad \hat{\alpha} \sim N(\alpha, \sigma^{(\alpha)2})$$

For formulas of the standard deviations $\sigma^{(\beta)2}$ and $\sigma^{(\alpha)2}$, please consult Stahel 2.2.h.

To remember:

- $\hat{\alpha}$ and $\hat{\beta}$ are unbiased estimators of α and β.
- the parameters estimates $\hat{\alpha}$ and $\hat{\beta}$ are normally distributed.
- the formulas for the variances depend on the residual variance σ^2, the sample size n and the variability of X ($\text{SSQ}^{(X)(\star)}$).

$$\text{SSQ}^{(X)} \overset{(\star)}{=} \sum_{i=1}^{n} (x_i - \overline{x})^2$$

Are the modelling assumptions met?

In practice, it is advisable to check if all our modelling assumptions are met.

$\rightarrow$ Otherwise we might draw invalid conclusions from the results.

Remember: Our assumption is that $\epsilon_i \sim N(0, \sigma^2)$. This implies

a) The expected value of ϵ_i is 0: $E(\epsilon_i) = 0$.
b) All ϵ_i have the same variance: $Var(\epsilon_i) = \sigma^2$.
c) All ϵ_i are normally distributed.

In addition, it is assumed that

d) $\epsilon_1, \epsilon_2, \ldots, \epsilon_n$ are independent.

Note: We do not actually observe ϵ_i, but only the residuals e_i. Let us introduce two simple graphical model checking tools for our residuals e_i.