

# Linear regression and correlation

The ASTA team

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## 1 The regression problem

### 1.1 We want to predict

- We will study the dataset `trees`, which is on the course website (and actually also already available in R).

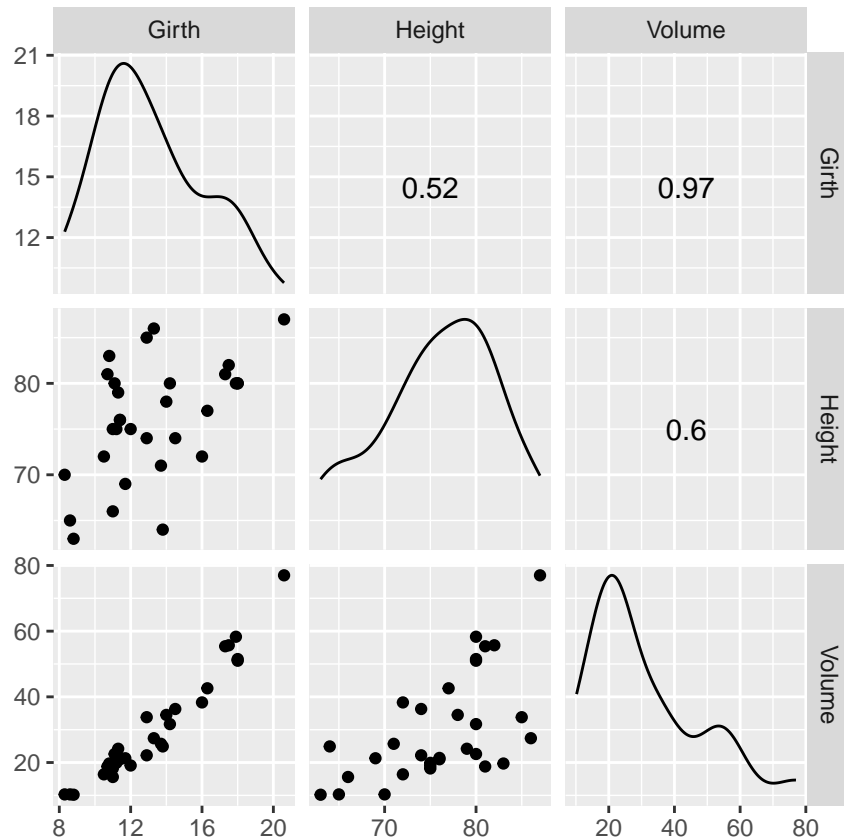
```
trees <- read.delim("https://asta.math.aau.dk/datasets?file=trees.txt")
```

- In this experiment we have measurements of 3 variables for 31 randomly chosen trees:
- `[,1]` `Girth` numeric. Tree diameter in inches.
- `[,2]` `Height` numeric. Height in ft.
- `[,3]` `Volume` numeric. Volume of timber in cubic ft.
- We want to predict the tree volume, if we measure the tree height and/or the tree girth (diameter).
- This type of problem is called **regression**.
- Relevant terminology:
  - We measure a quantitative **response**  $y$ , e.g. `Volume`.
  - In connection with the response value  $y$  we also measure one (later we will consider several) potential **explanatory** variable  $x$ . Another name for the explanatory variable is **predictor**.

### 1.2 Initial graphics

- Any analysis starts with relevant graphics.

```
library(mosaic)
library(GGally)
ggscatmat(trees) # Scatter plot matrix from GGally package
```



- For each combination of the variables we plot the  $(x, y)$  values.
- It looks like **Girth** is a good predictor for **Volume**.
- If we only are interested in the association between two (and not three or more) variables we use the usual `gf_point` function.

### 1.3 Simple linear regression

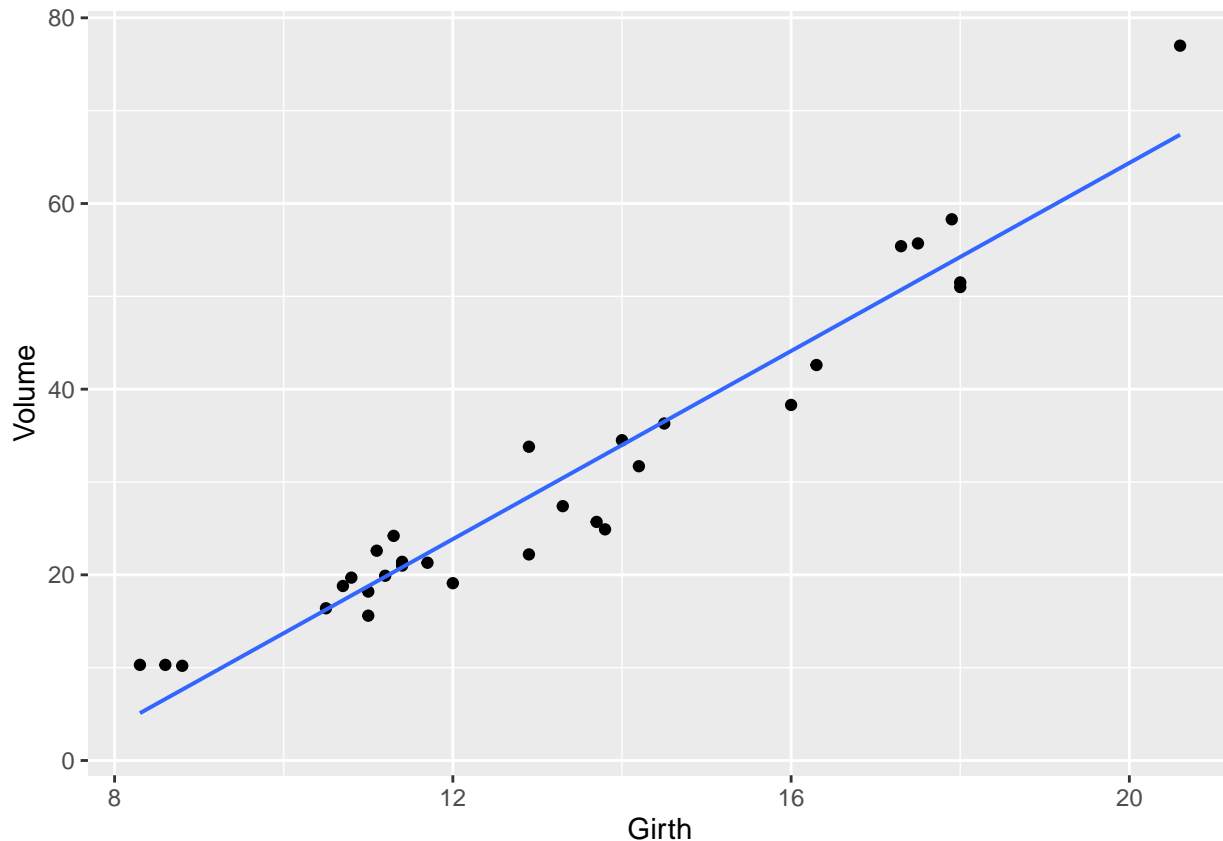
- We choose to use  $x$ =**Girth** as predictor for  $y$ =**Volume**. When we only use one predictor we are doing **simple regression**.
- The simplest **model** to describe an association between **response**  $y$  and a **predictor**  $x$  is **simple linear regression**.
- I.e. ideally we see the picture

$$y(x) = \alpha + \beta x$$

where

- $\alpha$  is called the **Intercept** - the line's intercept with the  $y$ -axis, corresponding to the response for  $x = 0$ .
- $\beta$  is called **Slope** - the line's slope, corresponding to the change in response, when we increase the predictor by one unit.

```
gf_point(Volume ~ Girth, data = trees) %>% gf_lm()
```



## 1.4 Model for linear regression

- Assume we have a sample with joint measurements  $(x, y)$  of predictor and response.
- Ideally the model states that

$$y(x) = \alpha + \beta x,$$

but due to random variation there are deviations from the line.

- What we observe can then be described by

$$y = \alpha + \beta x + \varepsilon,$$

where  $\varepsilon$  is a **random error**, which causes deviations from the line.

- We will continue under the following **fundamental assumption**:
  - The errors  $\varepsilon$  are normally distributed with mean zero and standard deviation  $\sigma_{y|x}$ .
- We call  $\sigma_{y|x}$  the **conditional standard deviation** given  $x$ , since it describes the variation in  $y$  around the regression line, when we know  $x$ .

## 1.5 Least squares

- In summary, we have a model with 3 parameters:
  - $(\alpha, \beta)$  which determine the line
  - $\sigma_{y|x}$  which is the standard deviation of the deviations from the line.
- How are these estimated, when we have a sample  $(x_1, y_1) \dots (x_n, y_n)$  of  $(x, y)$  values??
- To do this we focus on the errors

$$\varepsilon_i = y_i - \alpha - \beta x_i$$

which should be as close to 0 as possible in order to fit the data best possible.

- We will choose the line, which minimizes the sum of squares of the errors:

$$\sum_{i=1}^n \varepsilon_i^2 = \sum_{i=1}^n (y_i - \alpha - \beta x_i)^2.$$

- If we set the partial derivatives to zero we obtain two linear equations for the unknowns  $(\alpha, \beta)$ , where the solution  $(a, b)$  is given by:

$$b = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^n (x_i - \bar{x})^2} \quad \text{and} \quad a = \bar{y} - b\bar{x}$$

## 1.6 The prediction equation and residuals

- The equation for the estimates  $(\hat{\alpha}, \hat{\beta}) = (a, b)$ ,

$$\hat{y} = a + bx$$

is called **the prediction equation**, since it can be used to predict  $y$  for any value of  $x$ .

- Note: The prediction equation is determined by the current sample. I.e. there is an uncertainty attached to it. A new sample would without any doubt give a different prediction equation.
- Our best estimate of the errors is

$$e_i = y_i - \hat{y} = y_i - a - bx_i,$$

i.e. the vertical deviations from the prediction line.

- These quantities are called **residuals**.
- We have that
  - The prediction line passes through the point  $(\bar{x}, \bar{y})$ .
  - The sum of the residuals is zero.

## 1.7 Estimation of conditional standard deviation

- To estimate  $\sigma_{y|x}$  we need **Sum of Squared Errors**

$$SSE = \sum_{i=1}^n e_i^2 = \sum_{i=1}^n (y_i - \hat{y}_i)^2,$$

which is the squared distance between the model and data.

- We then estimate  $\sigma_{y|x}$  by the quantity

$$s_{y|x} = \sqrt{\frac{SSE}{n-2}}$$

- Instead of  $n$  we divide  $SSE$  with **the degrees of freedom**  $df = n - 2$ . Theory shows, that this is reasonable.
- The degrees of freedom  $df$  are determined as the sample size minus the number of parameters in the regression equation.
- In the current setup we have 2 parameters:  $(\alpha, \beta)$ .

## 1.8 Example in R

```
model <- lm(Volume ~ Girth, data = trees)
summary(model)
```

```
##
## Call:
## lm(formula = Volume ~ Girth, data = trees)
##
## Residuals:
##   Min       1Q   Median       3Q      Max
## -8.065 -3.107  0.152  3.495  9.587
##
## Coefficients:
##           Estimate Std. Error t value Pr(>|t|)
## (Intercept) -36.9435     3.3651  -10.98 7.62e-12 ***
## Girth         5.0659     0.2474   20.48 < 2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 4.252 on 29 degrees of freedom
## Multiple R-squared:  0.9353, Adjusted R-squared:  0.9331
## F-statistic: 419.4 on 1 and 29 DF,  p-value: < 2.2e-16
```

- The estimated residuals vary from -8.065 to 9.578 with median 0.152.
- The estimate of **Intercept** is  $a = -36.9435$
- The estimate of slope of **Girth** is  $b = 5.0659$
- The estimate of the conditional standard deviation (called residual standard error in **R**) is  $s_{y|x} = 4.252$  with  $31 - 2 = 29$  degrees of freedom.

## 1.9 Test for independence

- We consider the regression model

$$y = \alpha + \beta x + \varepsilon$$

where we use a sample to obtain estimates  $(a, b)$  of  $(\alpha, \beta)$ , an estimate  $s_{y|x}$  of  $\sigma_{y|x}$  and the degrees of freedom  $df = n - 2$ .

- We are going to test

$$H_0 : \beta = 0 \quad \text{against} \quad H_a : \beta \neq 0$$

- The null hypothesis specifies, that  $y$  **doesn't** depend linearly on  $x$ .
- In other words the question is: Is the value of  $b$  far away from zero?
- It can be shown that  $b$  has standard error

$$se_b = \frac{s_{y|x}}{\sqrt{\sum_{i=1}^n (x_i - \bar{x})^2}}$$

with  $df$  degrees of freedom.

- So, we want to use the test statistic

$$t_{\text{obs}} = \frac{b}{se_b}$$

which has to be evaluated in a t-distribution with  $df$  degrees of freedom.

## 1.10 Example

- Recall the summary of our example:

```
summary(model)
```

```
##
## Call:
## lm(formula = Volume ~ Girth, data = trees)
```

```
##
## Residuals:
##   Min      1Q  Median      3Q      Max
## -8.065 -3.107  0.152  3.495  9.587
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
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## ---
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```

- As we noted previously  $b = 5.0659$  and  $s_{y|x} = 4.252$  with  $df = 29$  degrees of freedom.
- In the second column(Std. Error) of the `Coefficients` table we find  $se_b = 0.2474$ .
- The observed t-score (test statistic) is then

$$t_{\text{obs}} = \frac{b}{se_b} = \frac{5.0659}{0.2474} = 20.48$$

which also can be found in the third column(`t value`).

- The corresponding p-value is found in the usual way by using the t-distribution with 29 degrees of freedom.
- In the fourth column(`Pr(>|t|)`) we see that the p-value is less than  $2 \times 10^{-16}$ . This is no surprise since the t-score was way above 3.

## 1.11 Confidence interval for slope

- When we have both the standard error and the reference distribution, we can construct a confidence interval in the usual way:

$$b \pm t_{\text{crit}} se_b,$$

where the t-score is determined by the confidence level and we find this value using `qdist` in **R**.

- In our example we have 29 degrees of freedom and with a confidence level of 95% we get  $t_{\text{crit}} = \text{qdist}("t", 0.975, df = 29) = 2.045$ .
- If you are lazy (like most statisticians are):

```
confint(model)
```

```
##              2.5 %      97.5 %
## (Intercept) -43.825953 -30.060965
## Girth        4.559914   5.571799
```

- i.e. (4.56, 5.57) is a 95% confidence interval for the slope of `Girth`.

## 1.12 Correlation

- The estimated slope  $b$  in a linear regression doesn't say anything about the strength of association between  $y$  and  $x$ .
- `Girth` was measured in inches, but if we rather measured it in kilometers the slope is much larger: An increase of 1km in `Girth` yield an enormous increase in `Volume`.
- Let  $s_y$  and  $s_x$  denote the sample standard deviation of  $y$  and  $x$ , respectively.

- The corresponding t-scores

$$y_t = \frac{y}{s_y} \quad \text{and} \quad x_t = \frac{x}{s_x}$$

are independent of the chosen measurement scale.

- The corresponding prediction equation is then

$$\hat{y}_t = \frac{a}{s_y} + \frac{s_x}{s_y} b x_t$$

- i.e. **the standardized regression coefficient** (slope) is

$$r = \frac{s_x}{s_y} b$$

which also is called **the correlation** between  $y$  and  $x$ .

- It can be shown that:
  - $-1 \leq r \leq 1$
  - The absolute value of  $r$  measures the (linear) strength of dependence between  $y$  and  $x$ .
  - When  $r = 1$  all the points are on the prediction line, which has positive slope.
  - When  $r = -1$  all the points are on the prediction line, which has negative slope.
- To calculate the correlation in **R**:

```
cor(trees)
```

```
##           Girth    Height    Volume
## Girth  1.0000000 0.5192801 0.9671194
## Height 0.5192801 1.0000000 0.5982497
## Volume 0.9671194 0.5982497 1.0000000
```

- There is a strong positive correlation between **Volume** and **Girth** ( $r=0.967$ ).
- Note, calling `cor` on a `data.frame` (like `trees`) only works when all columns are numeric. Otherwise the relevant numeric columns should be extracted like this:

```
cor(trees[,c("Height", "Girth", "Volume")])
```

which produces the same output as above.

- Alternatively, one can calculate the correlation between two variables of interest like:

```
cor(trees$Height, trees$Volume)
```

```
## [1] 0.5982497
```

## 2 R-squared: Reduction in prediction error

### 2.1 R-squared: Reduction in prediction error

- We want to compare two different models used to predict the response  $y$ .
- Model 1: We do not use the knowledge of  $x$ , and use  $\bar{y}$  to predict any  $y$ -measurement. The corresponding prediction error is defined as

$$TSS = \sum_{i=1}^n (y_i - \bar{y})^2$$

and is called the **Total Sum of Squares**.

- Model 2: We use the prediction equation  $\hat{y} = a + bx$  to predict  $y_i$ . The corresponding prediction error is then the Sum of Squared Errors

$$SSE = \sum_{i=1}^n (y_i - \hat{y}_i)^2.$$

- We then define

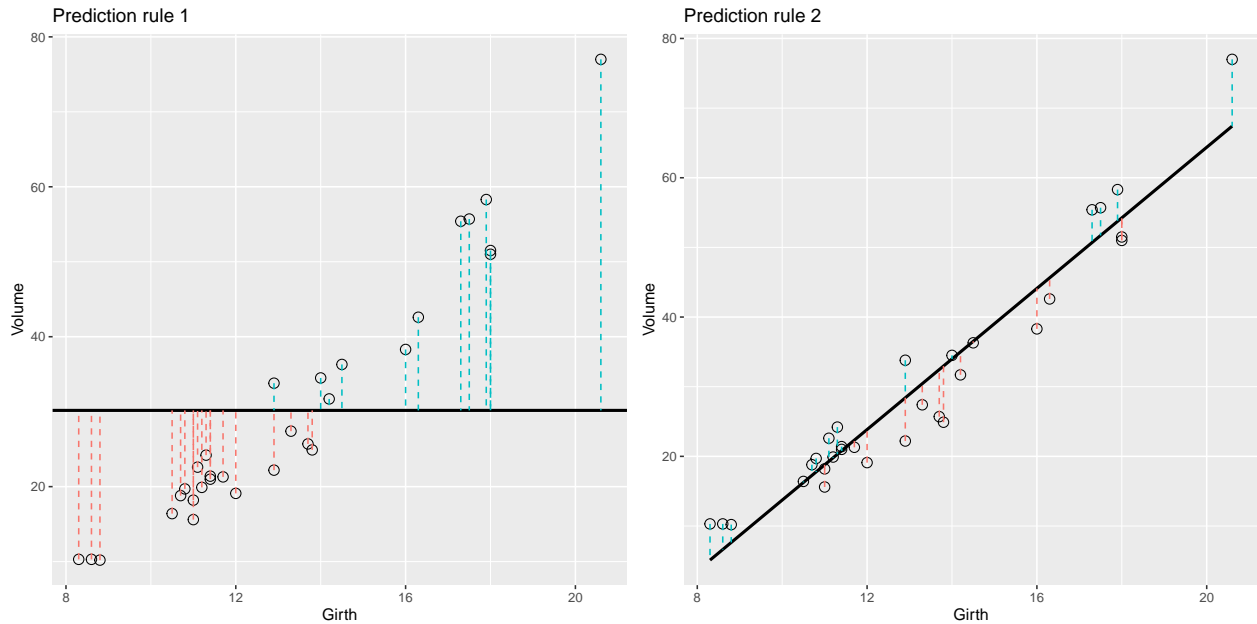
$$r^2 = \frac{TSS - SSE}{TSS}$$

which can be interpreted as the relative reduction in the prediction error, when we include  $x$  as explanatory variable.

- This is also called the **fraction of explained variation**, **coefficient of determination** or simply **r-squared**.
- For example if  $r^2 = 0.65$ , the interpretation is that  $x$  explains about 65% of the variation in  $y$ , whereas the rest is due to other sources of random variation.

## 2.2 Graphical illustration of sums of squares

```
## `geom_smooth()` using formula = 'y ~ x'
```



- Note the data points are the same in both plots. Only the prediction rule changes.
- The error of using Rule 1 is the total sum of squares  $E_1 = TSS = \sum_{i=1}^n (y_i - \bar{y})^2$ .
- The error of using Rule 2 is the residual sum of squares (sum of squared errors)  $E_2 = SSE = \sum_{i=1}^n (y_i - \hat{y}_i)^2$ .

## 2.3 $r^2$ : Reduction in prediction error

- For the simple linear regression we have that

$$r^2 = \frac{TSS - SSE}{TSS}$$

is equal to the square of the correlation between  $y$  and  $x$ , so it makes sense to denote it  $r^2$ .

- Towards the bottom of the output below we can read off the value  $r^2 = 0.9353 = 93.53\%$ , which is a large fraction of explained variation.

```
summary(model)
```

```
##
## Call:
## lm(formula = Volume ~ Girth, data = trees)
##
```



```

## Residuals:
##   Min      1Q  Median      3Q      Max
## -8.065 -3.107  0.152  3.495  9.587
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
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```