Linear regression and correlation

The ASTA team

Contents

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).

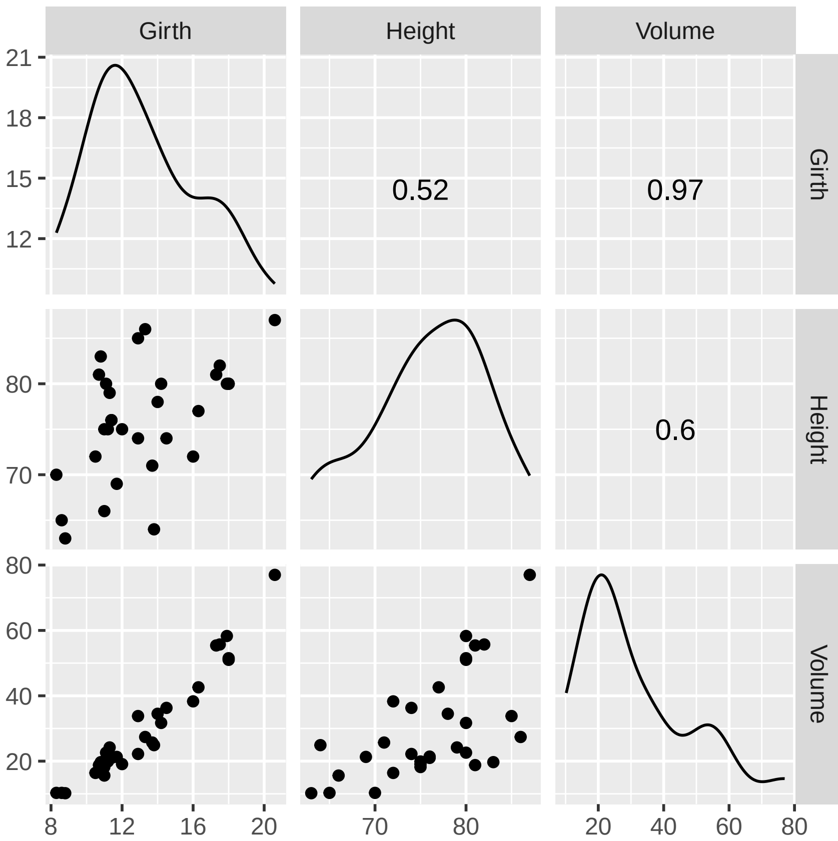
```
trees <- read.delim("https://asta.math.aau.dk/datasets?file=trees.txt")
```

- 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

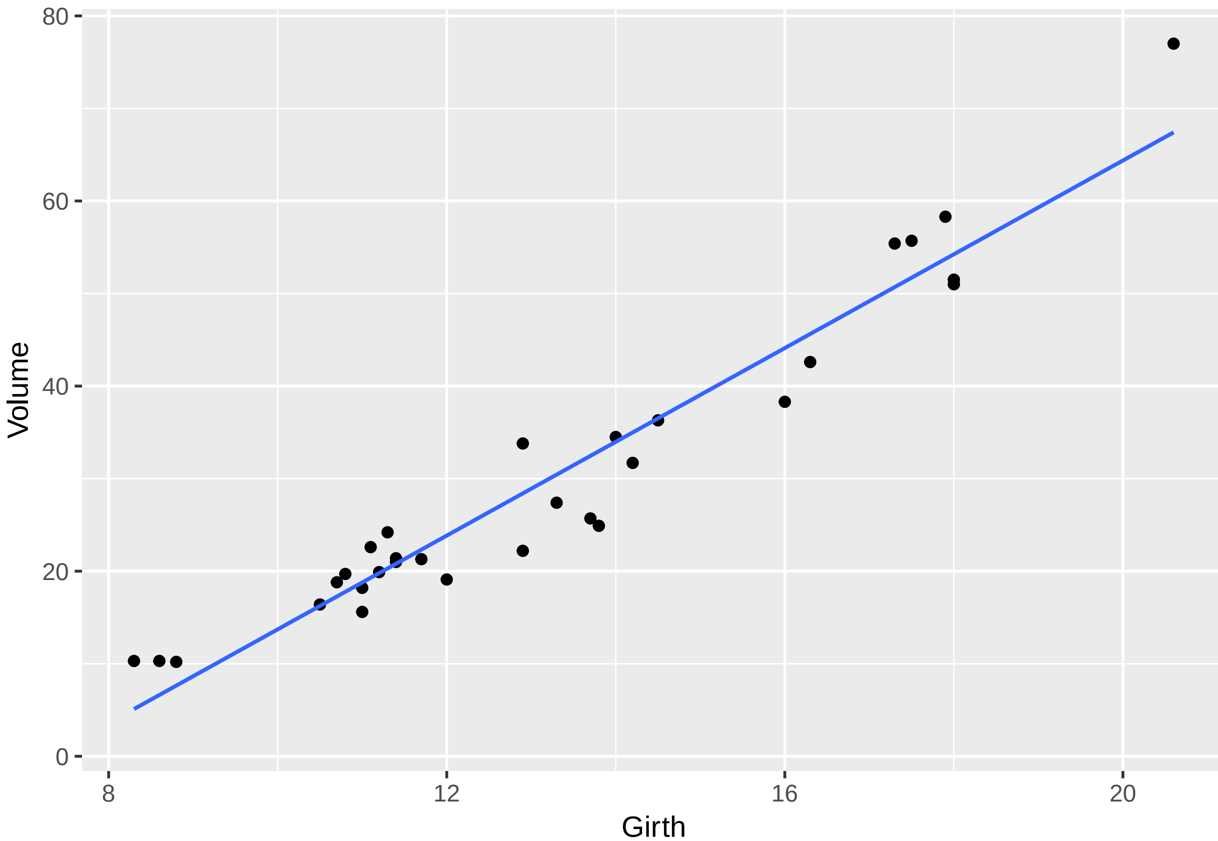
  $$y(x) = \alpha + \beta x$$

  where

  - α is called the `Intercept` - the line's intercept with the y-axis, corresponding to the response for $x = 0$.

- β 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 ε is a **random error**, which causes deviations from the line.
- We will continue under the following **fundamental assumption**:
  - The errors ε 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:

- (α, β) 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 $(x_1, y_1) \ldots (x_n, y_n)$ 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 chose 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 (α, β), 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: (α, β).

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 (α, β), 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:
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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 2×10^{-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:

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

  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 $t_{crit} =$ `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**:

```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:

```r
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:

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

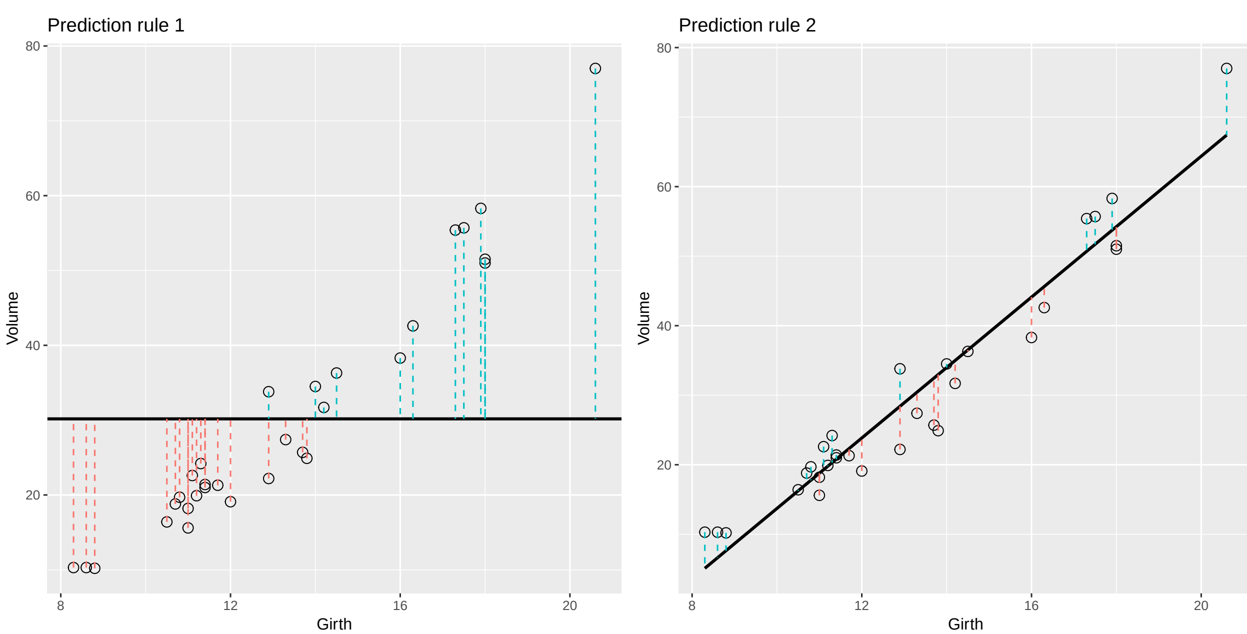
```
## [1] 0.5982497
```

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



- 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.

```r
summary(model)
```

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