# 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).

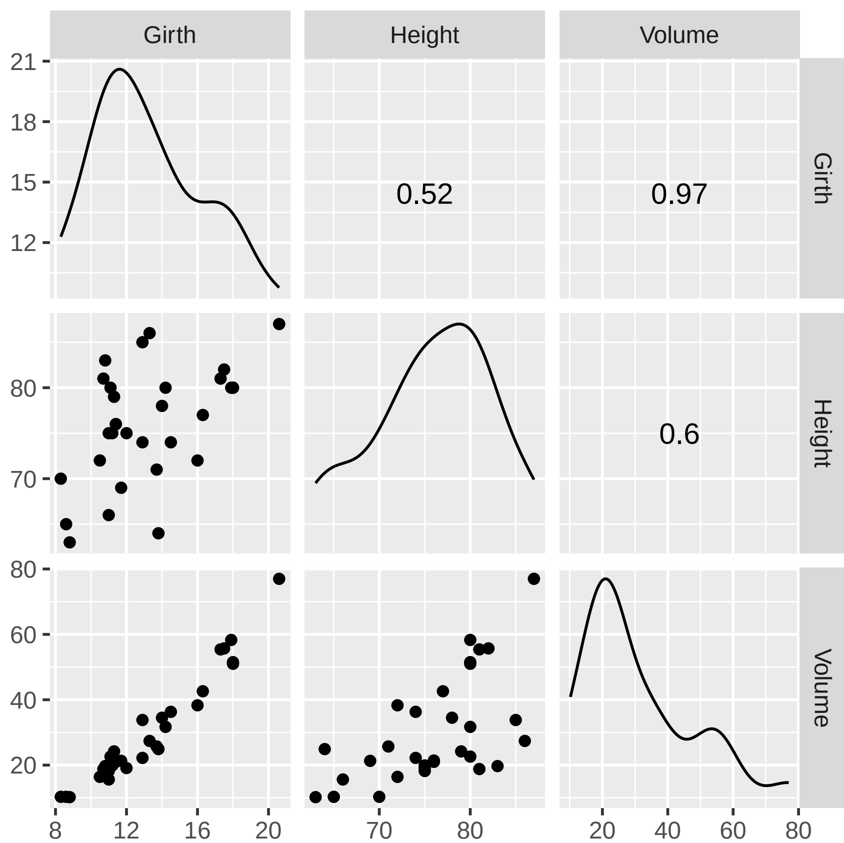
```r
trees <- read.delim("https://asta.math.aau.dk/datasets?file=trees.txt")
```

- In this experiment we have measurements of 3 variables for 31 randomly chosen trees:
- `Girth` numeric. Tree diameter in inches.
- `Height` numeric. Height in ft.
- `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.

```r
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

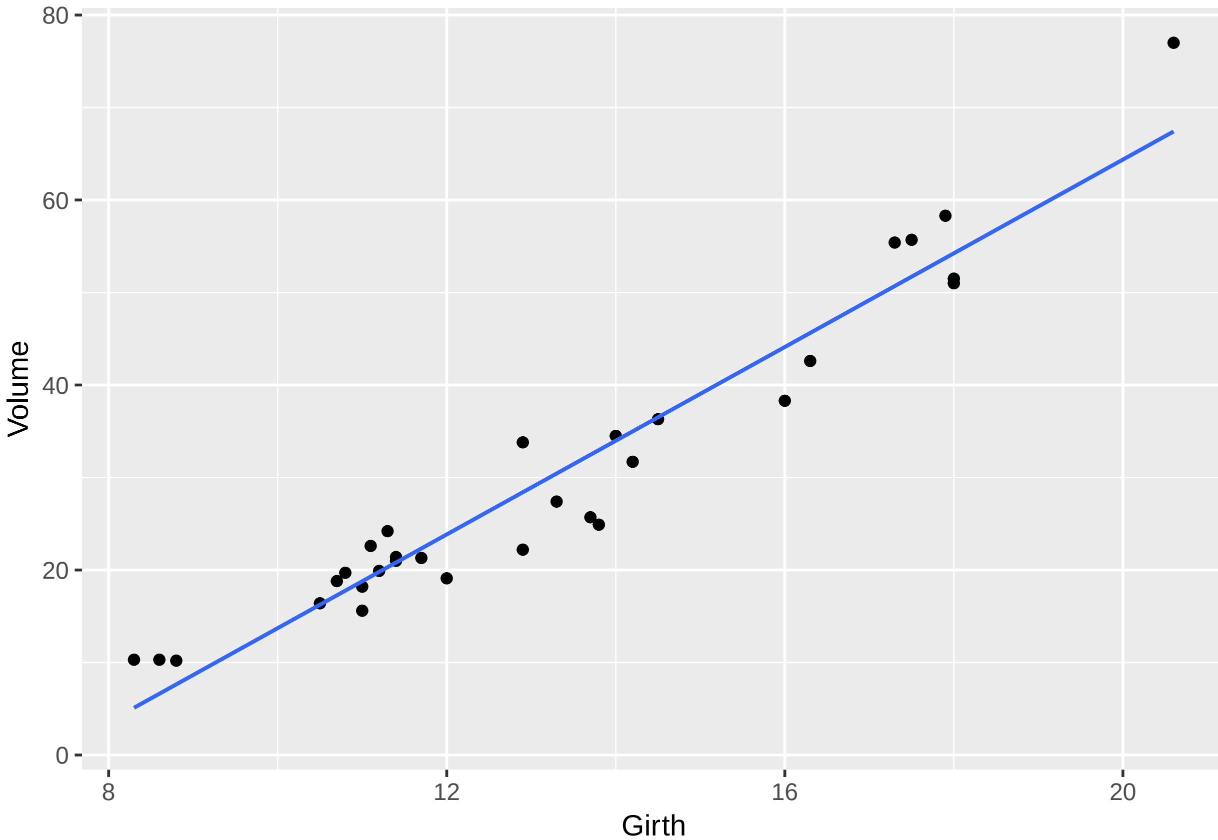
- We choose to use `x=Girth` as predictor for `y=Volume`. When we only use one predictor we are doing **simple regression**.
- The simplest **model** to describe an association between **response** $y$ and a **predictor** $x$ is **simple linear regression**.
- I.e. ideally we see the picture

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

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 $\sigma$.
- We call $\sigma$ 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
  - $\sigma$ 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 pairs 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 given by the estimates $(\hat{\alpha}, \hat{\beta}) = (a, b)$,

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

is called the **regression equation** or **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 $\sigma$ we need the **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 $\sigma$ by the quantity

$$s = \sqrt{\frac{SSE}{n-2}}$$

- 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 $s = 4.252$ 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 $(\alpha, \beta)$, the estimate $s$ of $\sigma$ 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 $x$.
- Observed values of $b$ far away from zero are critical for the null-hypothesis?
- It can be shown that $b$ has standard error
$$se_b = \frac{s}{\sqrt{\sum_{i=1}^{n}(x_i - \bar{x})^2}}$$
with $df = n - 2$ 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|)
## (Intercept) -36.9435     3.3651  -10.98 7.62e-12 ***
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## Residual standard error: 4.252 on 29 degrees of freedom
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```

- As we noted previously $b = 5.0659$ and $s = 4.252$ 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:

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

  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 (sample) correlation** between $y$ and $x$.

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- 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 sample 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

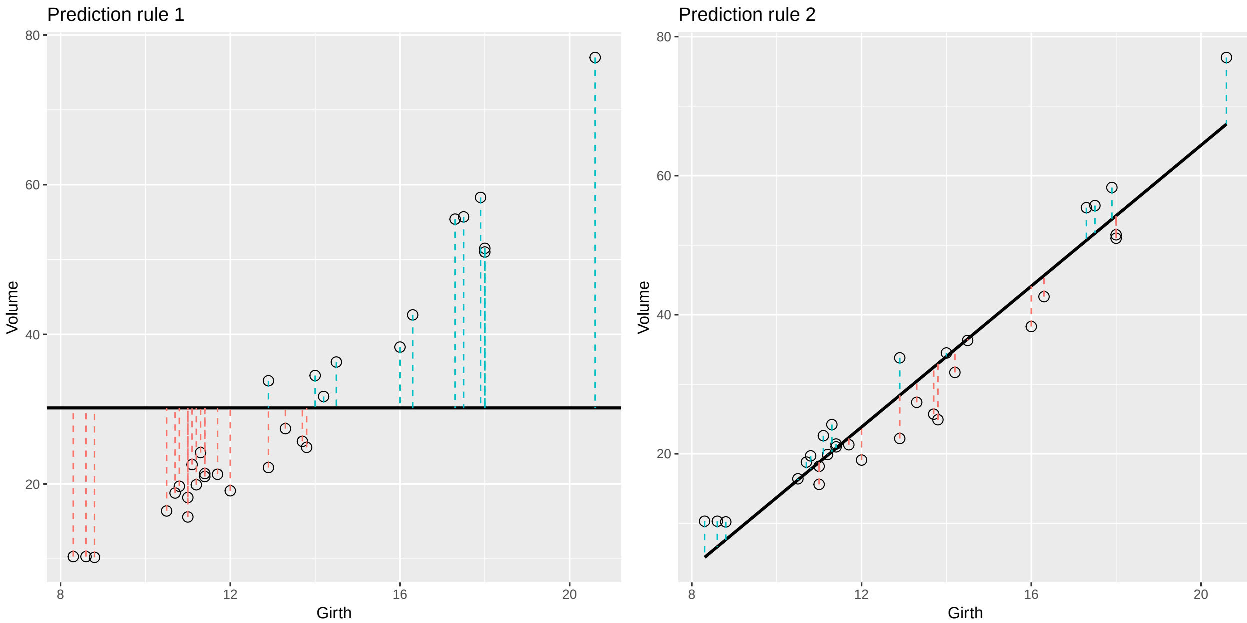
$$SSE = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2.$$

- 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




- 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|)
## (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
```

# 3 Introduction to multiple regression model

## 3.1 Multiple regression model

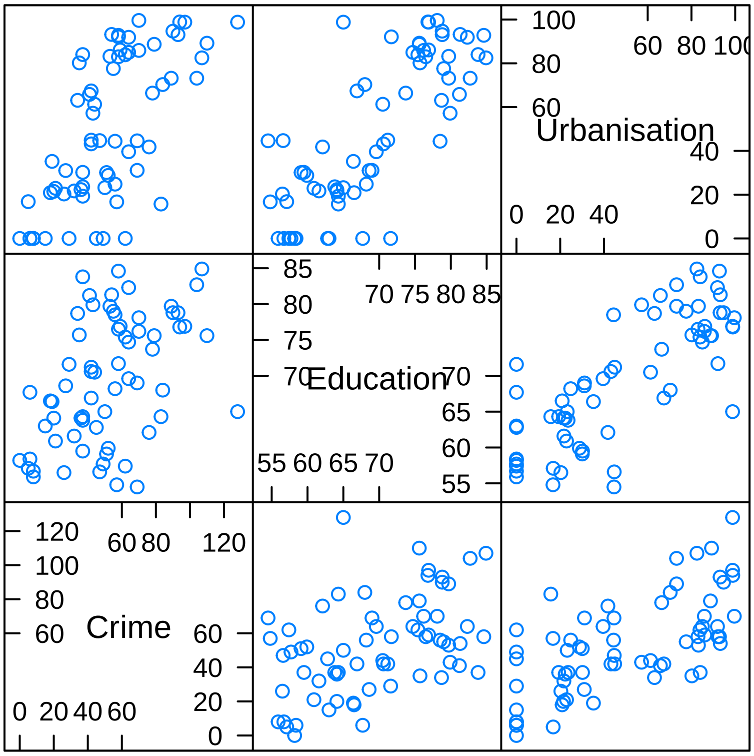
- We look at data set containing measurements from the 67 counties of Florida.
- Our focus is on
  - The response $y$: `Crime` which is the crime rate
  - The predictor $x_1$: `Education` which is proportion of the population with high school exam
  - The predictor $x_2$: `Urbanisation` which is proportion of the population living in urban areas

## 3.2 Example

```r
FL <- read.delim("https://asta.math.aau.dk/datasets?file=fl-crime.txt")
head(FL, n = 3)
```

```
##   Crime Education Urbanisation
## 1   104      82.7         73.2
## 2    20      64.1         21.5
## 3    64      74.7         85.0
```

```r
library(mosaic)
splom(FL) # Scatter PLOt Matrix
```




Scatter Plot Matrix

## 3.3 Correlations

- There is significant (p≈ $7 \times 10^{-5}$) positive correlation (r=0.47) between `Crime` and `Education`
- Then there is also significant positive correlation (r=0.68) between `Crime` and `Urbanisation`

```
cor(FL)
```

```
##                  Crime Education Urbanisation
## Crime        1.0000000 0.4669119    0.6773678
## Education    0.4669119 1.0000000    0.7907190
## Urbanisation 0.6773678 0.7907190    1.0000000
```

```
cor.test(~ Crime + Education, data = FL)
```

```
##
##  Pearson's product-moment correlation
##
## data:  Crime and Education
## t = 4.2569, df = 65, p-value = 6.806e-05
## alternative hypothesis: true correlation is not equal to 0
## 95 percent confidence interval:
##  0.2553414 0.6358104
## sample estimates:
##       cor
## 0.4669119
```

### 3.4 Several predictors

- Both `Education` ($x_1$) and `Urbanisation` ($x_2$) are pretty good predictors for `Crime` ($y$).
- We therefore want to consider the model

$$y = \alpha + \beta_1 x_1 + \beta_2 x_2 + \epsilon$$

- The errors $\epsilon$ are random noise with mean zero and standard deviation $\sigma$.
- The graph for the mean response is in other words a 2-dimensional plane in a 3-dimensional space.
- We determine estimates $(a, b_1, b_2)$ for $(\alpha, \beta_1, \beta_2)$ via the least squares method, i.e deviations from the plane.

### 3.5 Example

```
model <- lm(Crime ~ Education + Urbanisation, data = FL)
summary(model)
```

```
##
## Call:
## lm(formula = Crime ~ Education + Urbanisation, data = FL)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -34.693 -15.742  -6.226  15.812  50.678
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)   59.1181    28.3653   2.084   0.0411 *
## Education     -0.5834     0.4725  -1.235   0.2214
## Urbanisation   0.6825     0.1232   5.539 6.11e-07 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 20.82 on 64 degrees of freedom
## Multiple R-squared:  0.4714, Adjusted R-squared:  0.4549
## F-statistic: 28.54 on 2 and 64 DF,  p-value: 1.379e-09
```

- From the output we find the prediction equation

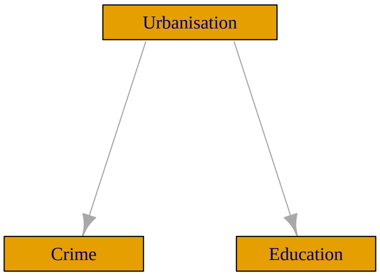
$$\widehat{y} = 59 - 0.58x_1 + 0.68x_2$$

- Not exactly what we expected based on the correlation.
- Now there appears to be a negative association between $y$ and $x_1$ (Simpsons Paradox)!
- We can also find the standard error (0.4725) and the corresponding t-score (-1.235) for the the slope of `Education`
- This yields a p-value of 22%, i.e. the slope is not significantly different from zero.

### 3.6 Simpsons paradox

- The example illustrates **Simpson's paradox**.
- When considered alone `Education` is a good predictor for `Crime` (with positive correlation).

- When we add `Urbanisation`, then `Education` has a negative effect on `Crime` (but not significant).




- A possible explanation is illustrated by the graph above.
  - `Urbanisation` has positive effect on both `Education` and `Crime`.
  - For a given level of `urbanisation` there is a (non-significant) negative association between `Education` and `Crime`.
  - Viewed alone `Education` is a good predictor for `Crime`. If `Education` has a large value, then this indicates a large value of `Urbanisation` and thereby a large value of `Crime`.