# Multiple linear regression <br> The ASTA team 

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## 1 Multiple regression model

### 1.1 Multiple regression model

- We look at data from Table 9.15 in Agresti. The data are measurements in 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


### 1.2 Example

FL <- read.delim("https://asta.math.aau.dk/datasets?file=fl-crime.txt") head $(\mathrm{FL}, \mathrm{n}=3)$

| \#\# | Crime | Education | Urbanisation |
| :--- | ---: | ---: | ---: |
| \#\# | 1 | 104 | 82.7 |
| \#\# 2 | 20 | 64.1 | 73.2 |
| \#\# 3 | 64 | 74.7 | 21.5 |

library (mosaic)
splom(FL) \# Scatter PLOt Matrix


### 1.3 Correlations

- There is significant ( $\mathrm{p} \approx 7 \times 10^{-5}$ ) positive correlation ( $\mathrm{r}=0.47$ ) 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
```


### 1.4 Several predictors

- Both Education $\left(x_{1}\right)$ and Urbanisation $\left(x_{2}\right)$ 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 $\sigma_{y \mid x}$.
- The graph for the mean response is in other words a 2-dimensional plane in 3-dimensional space.
- We determine estimates $\left(a, b_{1}, b_{2}\right)$ for $\left(\alpha, \beta_{1}, \beta_{2}\right)$ via the least squares method, i.e deviations from the plane.


### 1.5 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

$$
\widehat{y}=59-0.58 x_{1}+0.68 x_{2}
$$

- 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.


### 1.6 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.


## 2 The general model

### 2.1 Regression model

- We have a sample of size $n$, where we have measured
- the response $y$.
- $k$ potential predictors $x_{1}, x_{2}, \ldots, x_{k}$.
- Multiple regression model:

$$
y=\alpha+\beta_{1} x_{1}+\beta_{2} x_{2}+\ldots+\beta_{k} x_{k}+\epsilon
$$

- The errors $\epsilon$ are a sample from a population with mean zero and standard deviation $\sigma_{y \mid x}$.
- The systematic part of the model, i.e. when all errors are zero, says that the mean response is a linear function of the predictors:

$$
E\left(y \mid x_{1}, x_{2}, \ldots, x_{k}\right)=\alpha+\beta_{1} x_{1}+\beta_{2} x_{2}+\ldots+\beta_{k} x_{k}
$$

- The symbol $E$ is used here to denote expectation, i.e., mean value.


### 2.2 Interpretation of parameters

- In the multiple linear regression model

$$
E\left(y \mid x_{1}, x_{2}, \ldots, x_{k}\right)=\alpha+\beta_{1} x_{1}+\beta_{2} x_{2}+\ldots+\beta_{k} x_{k}
$$

- The parameter $\alpha$ is the Intercept, corresponding to the mean response, when all predictors are equal to zero.
- The parameters $\left(\beta_{1}, \beta_{2}, \ldots, \beta_{k}\right)$ are called partial regression coefficients.
- Imagine that alle predictors but $x_{1}$ are held fixed. Then $y=\tilde{\alpha}+\beta_{1} x_{1}$ is a line with slope $\beta_{1}$, which describes the rate of change in the mean response, when $x_{1}$ is changed one unit. Here

$$
\tilde{\alpha}=\alpha+\beta_{2} x_{2}+\cdots+\beta_{k} x_{k}
$$

is a constant number since we assumed all predictors but $x_{1}$ was held fixed.

- The rate of change $\beta_{1}$ does not depend on the value of the remaining predictors. In this case we say that there is no interaction between the effects of the predictors on the response.
- The above holds similarly for the other partial regression coefficients.
- An example of a model with interaction is

$$
E\left(y \mid x_{1}, x_{2}\right)=\alpha+\beta_{1} x_{1}+\beta_{2} x_{2}+\beta_{3} x_{1} x_{2}=\alpha+\beta_{2} x_{2}+\left(\beta_{1}+\beta_{3} x_{2}\right) x_{1}
$$

- When we fix $x_{2}$ the line has slope $\beta_{1}+\beta_{3} x_{2}$, which depends on the chosen value of $x_{2}$.


## 3 Estimation

### 3.1 Estimation of model

- The estimate $\left(a, b_{1}, b_{2}, \ldots, b_{k}\right)$ for $\left(\alpha, \beta_{1}, \beta_{2}, \ldots, \beta_{k}\right)$ is determined by minimizing the sum of squared errors.
- Based on this estimate we write the prediction equation as

$$
\widehat{y}=a+b_{1} x_{1}+b_{2} x_{2}+\ldots+b_{k} x_{k}
$$

- The distance between model and data is measured by the sum of squared erros

$$
S S E=\sum_{i=1}^{n} e_{i}^{2}=\sum_{i=1}^{n}\left(y_{i}-\widehat{y}_{i}\right)^{2}
$$

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

$$
s_{y \mid x}=\sqrt{\frac{S S E}{n-k-1}}
$$

- Rather than $n$ we divide $S S E$ by the degrees of freedom $d f=n-k-1$. Theory shows, that this is reasonable.
- The degrees of freedom $d f$ are determined by the sample size minus the number of parameters in the regression equation.
- Currently we have $k+1$ parameters: 1 intercept and $k$ slopes.


## 4 Multiple R-squared

### 4.1 Multiple $R^{2}$

- We want to compare two models to predict the response $y$. Analogous to simple linear regression we have the following setup:
- Model 1: We do not use the predictors, and use $\bar{y}$ to predict any $y$-measurement. The corresponding prediction error is
$-T S S=\sum_{i=1}^{n}\left(y_{i}-\bar{y}\right)^{2}$ and is called the Total Sum of Squares.
- Model 2: We use the multiple prediction equation to predict $y$, i.e. the prediction error is
$-S S E=\sum_{i=1}^{n}\left(y_{i}-\widehat{y}_{i}\right)^{2}$ and is called Sum of Squared Errors.
- We then define the multiple coefficient of determination

$$
R^{2}=\frac{T S S-S S E}{T S S}
$$

- Thus, $R^{2}$ is the relative reduction in prediction error, when we use $x_{1}, x_{2}, \ldots, x_{k}$ as explanatory variables.
- It can be shown that the multiple correlation $R=\sqrt{R^{2}}$ is the correlation between $y$ and $\widehat{y}$.

```
gf_point(predict(model) ~ FL$Crime) %>%
    gf_lm() %>%
    gf_labs(title = paste("Correlation between predicted and observed y ( r =", round(sqrt(summary(model)
            x = "Crime",
            y = expression(hat(y)))
```

Correlation between predicted and observed y ( $\mathrm{r}=0.69$ )


### 4.2 Example

```
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
```

- The prediction equation is $\widehat{y}=59-0.58 x_{1}+0.68 x_{2}$
- The estimate for $\sigma_{y \mid x}$ is $s_{y \mid x}=20.82$ (Residual standard error in $\mathbf{R}$ ) with $d f=67-3=64$ degrees of freedom.
- Multiple $R^{2}=0.4714$, i.e. $47 \%$ of the variation in the response is explained by including the predictors in the model.
- The estimate $b_{1}=-0.5834$ has standard error (Std. Error) se $=0.4725$ with corresponding $t$-score ( t value) $t_{\text {obs }}=\frac{-0.5834}{0.4725}=-1.235$.
- The hypothesis $H_{0}: \beta_{1}=0$ has the $t$-score $t_{\text {obs }}=-1.235$, which means that $b_{1}$ isn't significantly different from zero, since the $p$-value $(\operatorname{Pr}(>|\mathrm{t}|))$ is $22 \%$. That means that we should exclude Education as a predictor.


### 4.3 Example

- Our final model is then a simple linear regression:

```
model2 <- lm(Crime ~ Urbanisation, data = FL)
summary(model2)
##
## Call:
## lm(formula = Crime ~ Urbanisation, data = FL)
##
## Residuals:
## Min 1Q Median 3Q Max
## -34.766 -16.541 -4.741 16.521 49.632
##
## Coefficients:
## Estimate Std. Error t value Pr(>|t|)
## (Intercept) 24.54125 4.53930 5.406 9.85e-07 ***
```

```
## Urbanisation 0.56220 0.07573 7.424 3.08e-10 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 20.9 on 65 degrees of freedom
## Multiple R-squared: 0.4588, Adjusted R-squared: 0.4505
## F-statistic: 55.11 on 1 and 65 DF, p-value: 3.084e-10
```

- The coefficient of determination always decreases, when the model is simpler. Now we have $R^{2}=46 \%$, where before we had $47 \%$. But the decrease is not significant.


## 5 F-test for effect of predictors

### 5.1 F-test

- We consider the hypothesis

$$
H_{0}: \beta_{1}=\beta_{2}=\ldots=\beta_{k}=0
$$

against the alternative, that at least one of these are non-zero.

- As test statistic we use

$$
F_{o b s}=\frac{(n-k-1) R^{2}}{k\left(1-R^{2}\right)}
$$

- Large values of $R^{2}$ implies large values of $F$, which points to the alternative hypothesis.
- I.e. when we have calculated the observed value $F_{o b s}$, then we have to find the probability that a new experiment would result in a larger value.
- It can be shown that the reference distribution is (can be approximated by) a so-called $\mathbf{F}$-distribution with degrees of freedom $d f_{1}=k$ and $d f_{2}=n-k-1$.


### 5.2 Example

- We return to Crime and the prediction equation $\widehat{y}=59-0.58 x_{1}+0.68 x_{2}$, where $n=67$ and $R^{2}=0.4714$. We have
$-d f_{1}=k=2$ since we have 2 predictors.
$-d f_{2}=n-k-1=67-2-1=64$.
- Then we can calculate $F_{o b s}=\frac{(n-k-1) R^{2}}{k\left(1-R^{2}\right)}=28.54$
- To evaluate the value 28.54 in the relevant F-distribution:

1 - pdist("f", 28.54, df1=2, df2=64)

\#\# [1] 1.378612e-09

- So $p$-value $=1.38 \times 10^{-9}$ (notice we don't multiply by 2 since this is a one-sided test; only large values point more towards the alternative than the null hypothesis).
- All this can be found in the summary output we already have:

```
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
```


## 6 Test for interaction

### 6.1 Interaction between effects of predictors

- Could it be possible that a combination of Education and Urbanisation is good for prediction? We want to investigate this using the model

$$
E\left(y \mid x_{1}, x_{2}\right)=\alpha+\beta_{1} x_{1}+\beta_{2} x_{2}+\beta_{3} x_{1} x_{2}
$$

where we have extended with a possible effect of the product $x_{1} x_{2}$ :

```
model3 <- lm(Crime ~ Urbanisation * Education, data = FL)
summary(model3)
##
## Call:
## lm(formula = Crime ~ Urbanisation * Education, data = FL)
##
## Residuals:
## Min 1Q Median 3Q Max
## -35.181 -15.207 -6.457 14.559 49.889
##
## Coefficients:
## Estimate Std. Error t value Pr (>|t|)
## (Intercept) 19.31754 49.95871 0.387 0.700
## Urbanisation 1.51431 0.86809 1.744 0.086 .
## Education 0.03396 0.79381 0.043 0.966
## Urbanisation:Education -0.01205 0.01245 -0.968 0.337
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 20.83 on 63 degrees of freedom
## Multiple R-squared: 0.4792, Adjusted R-squared: 0.4544
## F-statistic: 19.32 on 3 and 63 DF, p-value: 5.371e-09
```

- When we look at the $p$-values in the table nothing is significant at the $5 \%$ level!
- But the F-statistic tells us that the predictors collectively have a significant prediction ability.
- Why has the highly significant effect of $x_{2}$ disappeared? Because the predictors $x_{1}$ and $x_{1} x_{2}$ are able to explain the same as $x_{2}$.
- Previously we only had $x_{1}$ as alternative explanation to $x_{2}$ - and that wasn't enough.
- The phenomenon is called multicollinearity and illustrates that we can have different models with equally good predictive properties.
- In this case we will choose the model with $x_{2}$ since it is simpler.
- However, in general it can be difficult to choose between models. For example, if both height and weight are good predictors of some response, but one of them can be left out, which one do we choose?

