# Predictive Modeling Series 1

#### Exercise 1.1

This exercise aims at carrying out a simple regression analysis for the data set constructed by Frank Anscombe. The data you need for this exercise is called **anscombe** and consists of four response variables  $y_i$  and four predictors  $x_i$ . Consider the four models  $Y_i^k = \beta_0^k + \beta_1^k \cdot X_i^k + \epsilon_i$  for k = 1, ..., 4.

a) Determine for all four models the intercept and the slope of the least squares regression line and their standard errors. Determine as well  $\hat{\sigma}$ .

#### **R**-Hint:

```
reg <- lm(anscombe$y1 ~ anscombe$x1)
```

b) Plot the regression line for all four models in a scatter plot. Comment your observations of the results in a) and b).

#### R-Hint:

```
plot (anscombe$x1, anscombe$y1, ylab = "Y1", xlab = "X1")
abline(reg) #add the regression line
```

#### Exercise 1.2

Prices of antique clocks: McClave and Benson collected data on the basis of auctions about age and price of antique clocks. You find them in the data file antique\_clocks.dat.

a) Display the data as a scatter plot (price vs. age) and describe their functional dependence. **R**-Hints:

```
ant_clo <- read.table(file = "antique_clocks.dat", sep = ";",
    header = T)
plot(price ~ age, data = ant_clo)</pre>
```

b) Use a linear model to describe the relationship between **price** and **age** and determine the estimated coefficients. **R**-Hints:

```
fit <- lm(price ~ age, data = ant_clo)
coef(fit) # exctracts estimated coefficient
summary(fit) # extracts a summary of the fit</pre>
```

c) Draw a regression line in the scatter plot in a). Comment on the results. **R**-Hints:

```
abline(fit)
```

#### Exercise 1.3

An engineer intends to carry out an analysis of a windmill used for power generation. He collects data about the produced current (in Ampere) at different wind speeds (meter per second). You'll find the data in the file windmill.dat. (Source: Montgomery and Peck, Introduction to Linear Regression Analysis, Wiley.)

a) Generate a scatter plot (current (y-axis) vs. wind speed) and another scatter plot (current vs.  $\frac{1}{\text{wind speed}}$ ). What do you observe? **R**-Hints:

```
windmill <- read.table("windmill.dat", header = T)
windmill$x <- 1/windmill$wind_speed
par(mfrow = c(1, 2)) # two plots within one graphics
plot(current ~ wind_speed, data = windmill)
plot(current ~ x, data = windmill)</pre>
```

b) Use the least squares method to fit the model

current 
$$\approx \beta_0 + \beta_1 x$$
 with  $x = \frac{1}{\text{wind speed}}$ 

Determine the corresponding estimated coefficients and standard errors.

c) Determine a 99 % confidence interval for  $\beta_1$ . **R**-Hints:

```
confint (windmill_lm, parm = 2, level = 0.99)
```

- d) Generate a scatter plot (current vs. wind speed). How do you interpret the coefficients  $\beta_0$  and  $\beta_1$  in these plots ?
  - **Hint**: Let the wind speed approach infinity to interpret  $\beta_0$  and set the current to zero in order to interpret  $\beta_1$ . A sketch may be useful.
- e) Determine the expected value, a 95% confidence interval for the expected current and a 95% prediction interval at wind speeds of  $1\frac{m}{s}$  and  $10\frac{m}{s}$ . Comment on the results. **R**-Hints:

```
wm_new <- data.frame(x = c(1, 10))
```

Expected value along with confidence interval:

Predicted value along with prediction interval:

#### Exercise 1.4

In the middle of the 19th century, Scottish physicist James D. Forbes worked on a method to determine the altitude using the boiling point of water. It was known that the altitude can be determined by means of the air pressure. That is the reason why Forbes was interested in a relation between the boiling point of water and the air pressure. The data for this exercise originates from his work published in 1857. **Forbes.dat** contains the boiling point **y** (in Fahrenheit) and the air **pressure** (in inch of mercury) at 17 places in the Alps and in Scotland. (Source: S. Weisberg, *Applied Linear Regression*, Wiley (1985), p. 3)

- a) Add the variable  $\mathbf{x} = 100 \cdot \log(\mathbf{pressure})$  to the data frame **Forbes** and plot  $\mathbf{y}$  versus **pressure** and  $\mathbf{y}$  versus  $\mathbf{x}$ . Comment on your observations with respect to the two plots.
- b) Use a least squares fit to determine the regression line for **y** versus **x**. Have a look at the regression line in the scatter plot and describe your observations of the result.
- c) Use a least squares fit to determine the regression line for  $\mathbf{y}$  versus  $\mathbf{x}$ , but now omit the 12th observation. Compare the values  $\hat{\beta}_0$ ,  $\hat{\beta}_1$ ,  $\operatorname{se}(\hat{\beta}_0)$ ,  $\operatorname{se}(\hat{\beta}_1)$  and  $\hat{\sigma}$  with the ones you have found in part b).

#### **R**-Hints:

```
fit2 <- lm(y ~ x, data=Forbes[-12,])
% or
fit2 <- lm(y ~ x, data=Forbes, subset=-12)</pre>
```

In the following exercises, we keep the 12th observation omitted.

d) Test  $H_0: \beta_1 = 0$  versus  $H_A: \beta_1 \neq 0$  in the model  $Y_i = \beta_0 + x_i + \epsilon_i$  using the output of the regression analysis at the 5%-level.

- e) Determine a 95 %-confidence interval for the slope  $\beta_1$ .
- f) Determine the expected value of Y given the predictor value  $x_0 = 100 \cdot \log(26) = 325.81$ . Determine a 95 % and a 99 % confidence interval for  $E[Y|x_0]$ . *Voluntary exercise*: Plot a 99 % confidence band in the scatter plot.
- g) Determine a 99 % prediction interval for the observed value of Y for  $x_0 = 325.81$ . Compare this interval with the confidence interval you have found in exercise f).

#### Exercise 1.5

We would like to simulate the distribution of the estimated coefficient values  $\beta_0$  and  $\beta_1$ . Our model is  $Y_i = 4 + 2x_i + \epsilon_i$  with the following  $x_i$  values:

The measurement errors  $\epsilon_i$  are normally distributed with  $\mu = 0$  and  $\sigma^2 = 2$ .

a) Simulate the 10 values of  $Y_i$  on the basis of the model  $Y_i = 4 + 2x_i + \epsilon_i$  one hundred times and estimate the values of the regression coefficients  $\beta_0$  and  $\beta_1$ .

#### **R**-Hint, Simulation:

```
x_sim <- c(0,3,4,8,10,11,13,16,17,20)
error_sim <- matrix(rnorm(10*?, mean=?, sd=?), ncol=??)
y_sim <- 4 + 2*x_sim + error_sim
coef <- matrix(0, ncol=2, nrow=100) # Initialisieren
for(i in 1:?) coef[i,] <- coef(lm(y_sim[,i] ~ x_sim))</pre>
```

- b) Have a look at the distribution of the estimated regression coefficients by means of a histogram and a normal plot. Comment on your observations. Have a look at the joint distribution of the regression coefficients by means of a scatter plot.
- c) Determine the mean value of the 100 estimations of  $\beta_0$  and  $\beta_1$ . Determine as well their variance. Compare the results with the theoretical values.

## **Result Checker**

#### **E 1.4**:

- e) [0.4813, 0.4930]
- f) [205.099, 205.246] and [205.070, 205.275]
- g) [204.780, 205.566]

# **Predictive Modeling**

### **Solutions to Series 1**

#### Solution 1.1

a) The coefficients entering the linear models are determined by means of the R-functions lm() and summary().

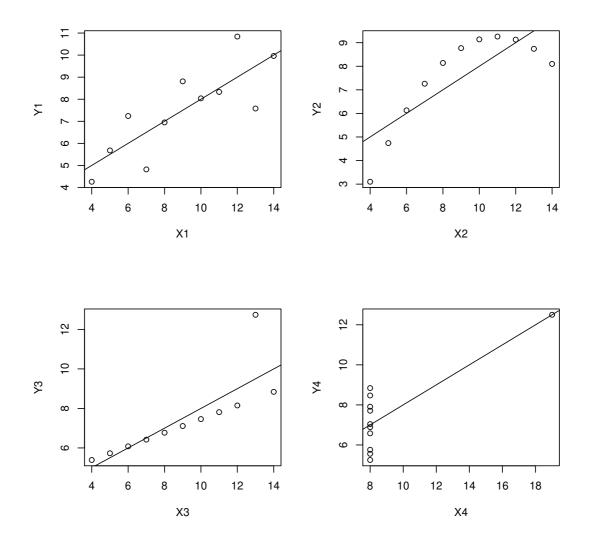
```
data (anscombe)
reg <- lm(anscombe$y1 ~ anscombe$x1)</pre>
reg2 <- lm(anscombe$y2 ~ anscombe$x2)</pre>
reg3 <- lm(anscombe$y3 ~ anscombe$x3)
reg4 <- lm(anscombe$y4 ~ anscombe$x4)
summary(reg) #analogous for the other models
##
## Call:
## lm(formula = anscombe$y1 ~ anscombe$x1)
##
## Residuals:
      Min
                 1Q Median
                                    3Q
                                            Max
## -1.92127 -0.45577 -0.04136 0.70941 1.83882
## Coefficients:
             Estimate Std. Error t value Pr(>|t|)
## (Intercept) 3.0001 1.1247 2.667 0.02573 *
## anscombe$x1 0.5001
                          0.1179 4.241 0.00217 **
## ---
## Signif. codes:
## 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 1.237 on 9 degrees of freedom
## Multiple R-squared: 0.6665, Adjusted R-squared: 0.6295
## F-statistic: 17.99 on 1 and 9 DF, p-value: 0.00217
```

The intercept  $\beta_0$  and the slope  $\beta_1$  are almost identical in all four models (see table).

Even the standard errors and  $\hat{\sigma}$  are very similar (1. model: standard error of  $\beta_0 = 1.125$ , standard error of  $\beta_1 = 0.117$  and residual standard error: 1.237).

	model 1	model 2	model 3	model 4
intercept $(\hat{\beta}_0)$	3.000	3.001	3.002	3.002
slope $(\hat{\beta}_1)$	0.500	0.500	0.500	0.500

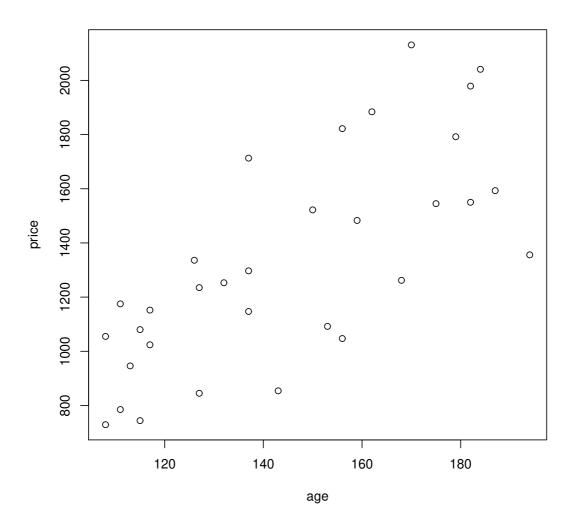
```
b) par(mfrow = c(2, 2))
  plot(anscombe$x1, anscombe$y1, ylab = "Y1", xlab = "X1")
  abline(reg)
  plot(anscombe$x2, anscombe$y2, ylab = "Y2", xlab = "X2")
  abline(reg2)
  plot(anscombe$x3, anscombe$y3, ylab = "Y3", xlab = "X3")
  abline(reg3)
  plot(anscombe$x4, anscombe$y4, ylab = "Y4", xlab = "X4")
  abline(reg4)
```



**Conclusion:** It is not sufficient to simply consider  $\hat{\beta}_0$ ,  $\hat{\beta}_1$  and their standard errors. These estimates are almost identical in every model, although the data are completely different. A (graphical) check is essential. Due to the similarity between the values of those coefficients, it is obvious that the regression lines are similar as well.

#### Solution 1.2

```
##
    1st Qu.:117.0
                     1st Qu.:1053
##
    Median :140.0
                     Median :1258
##
    Mean
           :144.9
                     Mean
                            :1327
    3rd Qu.:168.5
                     3rd Qu.:1561
##
##
    Max. :194.0
                     Max. :2131
plot (price ~ age, data = ant_clo)
```



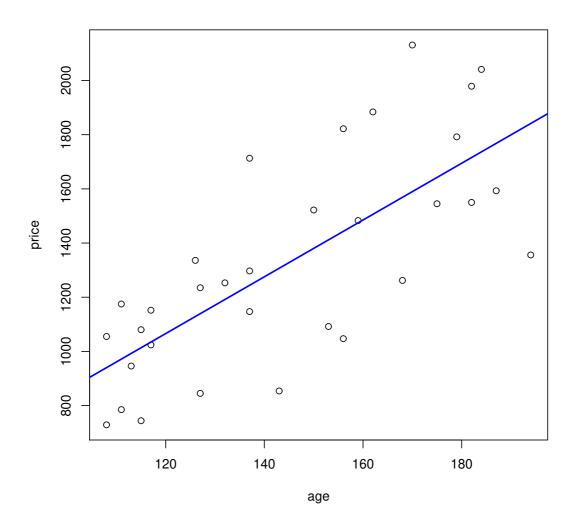
We observe a relatively strong variation in the data. However a linear trend can be observed: the older the clock, the more expensive it is.

```
b) ant_clo_fit <- lm(price ~ age, data = ant_clo)
summary(ant_clo_fit) # summary of the fit
##</pre>
```

```
## Call:
## lm(formula = price ~ age, data = ant_clo)
##
## Residuals:
## Min 1Q Median 3Q Max
## -485.29 -192.66 30.75 157.21 541.21
##
## Coefficients:
## Estimate Std. Error t value Pr(>|t|)
## (Intercept) -191.66 263.89 -0.726 0.473
               10.48
                          1.79 5.854 2.1e-06 ***
## age
## ---
## Signif. codes:
## 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 273 on 30 degrees of freedom
## Multiple R-squared: 0.5332, Adjusted R-squared: 0.5177
## F-statistic: 34.27 on 1 and 30 DF, p-value: 2.096e-06
```

The estimated coefficients are  $\hat{\beta}_0 = -191.66$  and  $\hat{\beta}_1 = 10.479$ . The residual standard Error is  $\hat{\sigma} = 273.028$ 

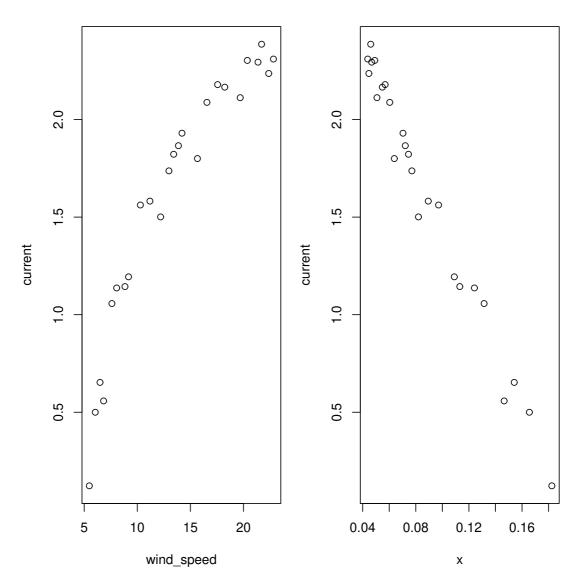
```
c) plot (price ~ age, data = ant_clo)
abline (ant_clo_fit, col = "blue", lwd = 2)
```



The regression line fits the data quite well.

#### Solution 1.3

```
a) d_dir <- "Daten/"
  windmill <- read.table(paste(d_dir, "windmill.dat", sep = ""),
        header = T)
  windmill$x <- 1/windmill$wind_speed
  par(mfrow = c(1, 2), mar = c(4, 4, 1, 1))
  plot(current ~ wind_speed, data = windmill)
  plot(current ~ x, data = windmill)</pre>
```



The regression line in the second scatter plot (current vs. x) seems to describe data better as compared to the first one.

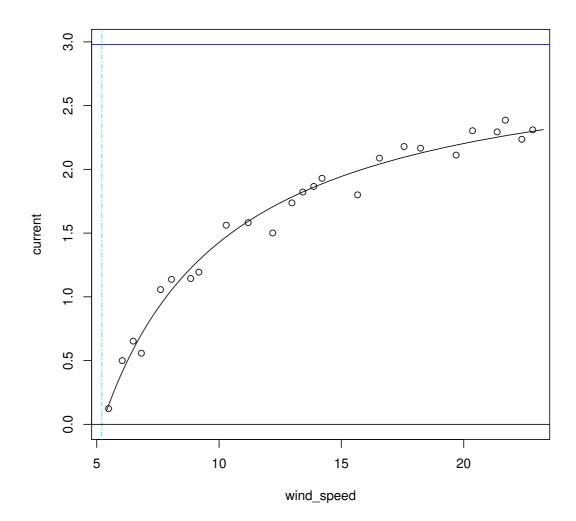
```
b) windmill_lm <- lm(current ~ x, data = windmill)
summary(windmill_lm)

##
## Call:
## lm(formula = current ~ x, data = windmill)
##
## Residuals:
## Min 1Q Median 3Q Max
## -0.20547 -0.04940 0.01100 0.08352 0.12204
##</pre>
```

```
## Coefficients:
## Estimate Std. Error t value Pr(>|t|)
## (Intercept) 2.9789 0.0449 66.34 <2e-16 ***
## x -15.5155 0.4619 -33.59 <2e-16 ***
## ---
## Signif. codes:
## 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.09417 on 23 degrees of freedom
## Multiple R-squared: 0.98, Adjusted R-squared: 0.9792
## F-statistic: 1128 on 1 and 23 DF, p-value: < 2.2e-16</pre>
```

The coefficients are  $\hat{\beta}_0 = 2.979$  and  $\hat{\beta}_1 = -15.515$ . The standard errors are  $\operatorname{se}(\hat{\beta}_0) = 0.0449$  and  $\operatorname{se}(\hat{\beta}_1) = 0.462$ .

$$lty = 6)$$
**abline**(h = 0)



The model is

current 
$$\approx \beta_0 + \beta_1 \frac{1}{\text{wind speed}}$$

As the wind speed approaches infinity,  $\beta_0$  becomes the maximally accessible current production (horizontal blue line).

The coefficient  $\beta_1$  is harder to interpret. It refers to the wind speed, at which the windmill starts to produce an electrical current at all:

$$0 = \beta_0 + \beta_1 \frac{1}{\text{windspeed}_0}$$

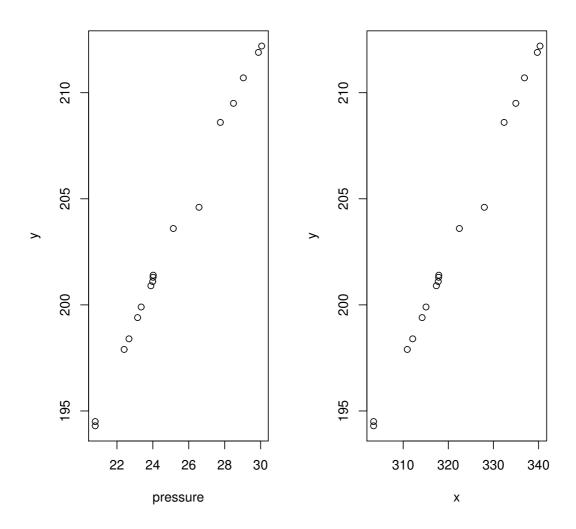
windspeed<sub>0</sub> = 
$$-\frac{\beta_1}{\beta_0}$$

This means, the larger the absolute value of  $\beta_1$  the larger the wind speed has to be, in order to have a windmill producing power.

Expected value with prediction interval:

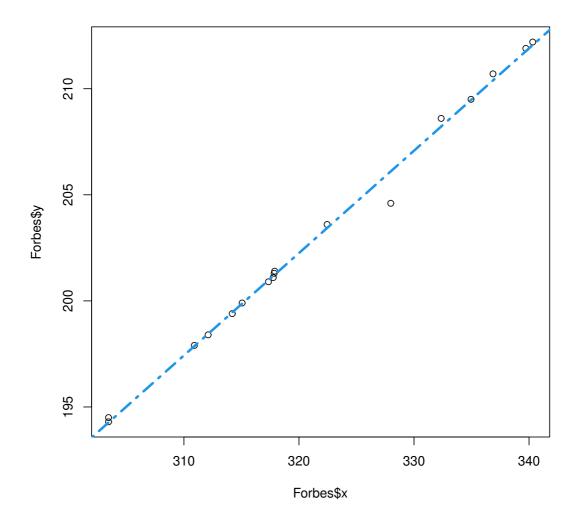
For the speed of  $10\frac{\text{m}}{\text{S}}$  we obtain a value of 1.43 A. As expected, the prediction intervals are (slightly) larger than the confidence intervals. The results for a wind speed of one meter per second do not make sense, because the wind-mill does not yet rotate (see exercise before). This problem arises because of the extrapolation of the model, which in this case is obviously non-sense.

#### Solution 1.4



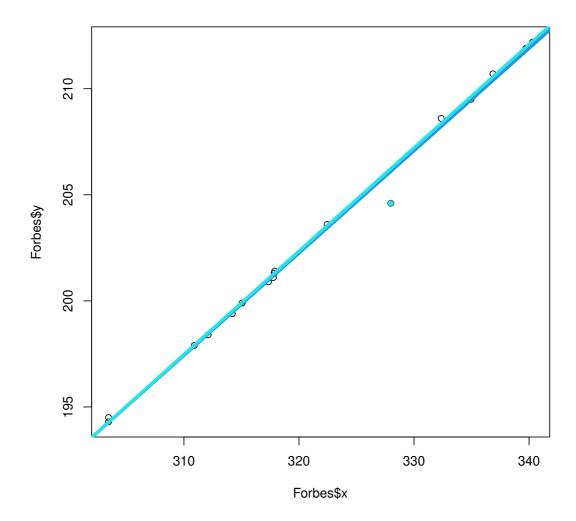
If we have a thorough look at the plot, we observe that data points in the first scatter plot lie on a slightly curved line. In the second scatter plot we observe that data points scatter almost perfectly around a straight line.

```
##
## Coefficients:
             Estimate Std. Error t value Pr(>|t|)
## (Intercept) 47.863838 2.851689 16.78 3.93e-11 ***
             ## X
## ---
## Signif. codes:
## 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.4223 on 15 degrees of freedom
## Multiple R-squared: 0.995, Adjusted R-squared: 0.9946
## F-statistic: 2962 on 1 and 15 DF, p-value: < 2.2e-16
par(mfrow = c(1, 1))
plot (Forbes$x, Forbes$y)
abline(Forbes_lm, col = 4, lty = 6, lwd = 3)
```



The above regression line fits data rather well, although an outlier is clearly visible - we can identify this point by means of the **R**-function **identify()**: it is the 12th observation.

```
c) plot (Forbes$x, Forbes$y)
points (Forbes$x[12], Forbes$y[12], col = 5, pch = 16)
abline (Forbes_lm, col = 4, lwd = 4)
ForbesR_lm <- lm(y ~ x, data = Forbes[-12, ])
# or
ForbesR_lm <- lm(y ~ x, data = Forbes, subset = -12)
abline (ForbesR_lm, col = 5, lty = 1, lwd = 4)</pre>
```



The **residual standard error** and the **standard errors** are reduced by a factor of 3.

In the following exercises we keep the 12th observation omitted.

d) Because the p-value of  $\beta_1$  is smaller than 0.05 (=significance level), the null-hypothesis  $\beta_1 = 0$  has to be rejected; i.e.  $\beta_1$  is significantly different from 0 at the 5% level.

```
e) confint (ForbesR_lm, parm = 2, level = 0.95)
## 2.5 % 97.5 %
## x 0.4813568 0.4929508
```

A 95 %-confidence interval for the slope  $\beta_1$  is given by [0.481, 0.493].

```
f) x0 < - data.frame (x = 325.81)
 predict (ForbesR_lm, newdata = x0)
  ##
           1
  ## 205.1726
 predict (ForbesR_lm, newdata = x0, interval = "confidence",
      level = 0.95)
            fit
                     lwr
                               upr
  ## 1 205.1726 205.0989 205.2463
 predict(ForbesR_lm, newdata = x0, interval = "confidence",
      level = 0.99)
            fit
                     lwr
 ## 1 205.1726 205.0703 205.2749
```

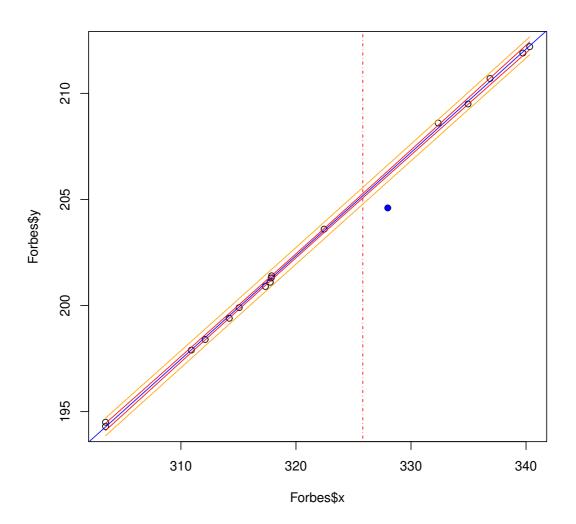
The expected value is 205.17. The confidence intervals are [205.099, 205.246] and [205.070, 205.275]. As expected, the 99 % confidence interval is larger than the 95 % interval.

A 99 %-prediction interval is [204.780, 205.566]. As expected, this interval is larger than the corresponding 99 %-confidence interval.

Voluntary Exercise:

```
plot (Forbes$x, Forbes$y)
points (Forbes$x[12], Forbes$y[12], col = "blue", pch = 16)
abline (ForbesR_lm, col = "blue", lty = 1)
abline (v = 325.81, lty = 4, col = "red")
x0 <- data.frame (x = seq(min(Forbes$x), max(Forbes$x), length = 50))
ForbesR.cia <- predict(ForbesR_lm, newdata = x0, interval = "confident level = 0.99)
ForbesR.pia <- predict(ForbesR_lm, newdata = x0, interval = "predict: level = 0.99)
lines(x0$x, ForbesR.cia[, "upr"], col = "red")
lines(x0$x, ForbesR.cia[, "lwr"], col = "red")
lines(x0$x, ForbesR.cia[, "upr"], col = "red")</pre>
```

```
lines(x0$x, ForbesR.pia[, "lwr"], col = "orange")
```



#### Solution 1.5

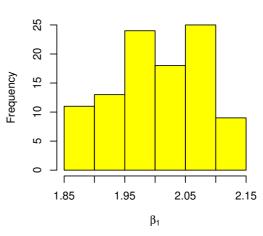
```
coef2 <- matrix(0, ncol = 2, nrow = 10000)
## Attention, this may take a while!
for (i in 1:10000) coef2[i, ] <- coef(lm(y_sim2[, i] ~ x_sim))

b) par(mfrow = c(2, 2))
hist(coef[, 1], xlab = expression(beta[0]), col = "blue")
hist(coef[, 2], xlab = expression(beta[1]), col = "yellow")
##
hist(coef2[, 1], xlab = expression(beta[0]), col = "blue")
hist(coef2[, 2], xlab = expression(beta[1]), col = "yellow")</pre>
```

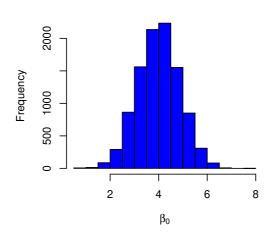
#### Histogram of coef[, 1]

# Ledneucy 2 3 4 5 6 β<sub>0</sub>

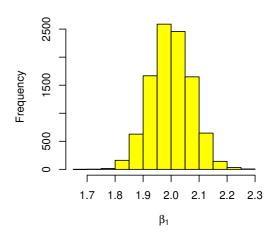
#### Histogram of coef[, 2]



#### Histogram of coef2[, 1]



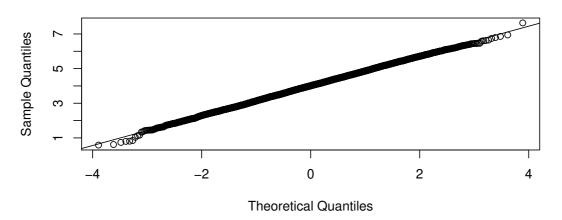
#### Histogram of coef2[, 2]



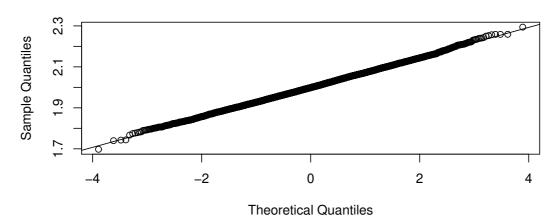
```
par (mfrow = c(2, 1))
qqnorm(coef2[, 1])
qqline(coef2[, 1])
```

```
##
qqnorm(coef2[, 2])
qqline(coef2[, 2])
```

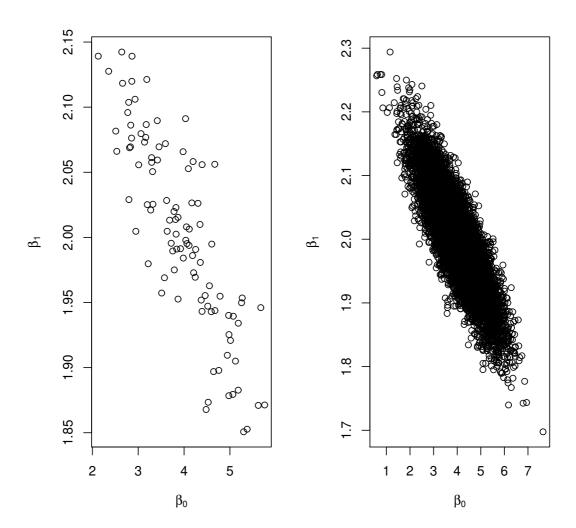
#### Normal Q-Q Plot



#### Normal Q-Q Plot



The following scatter plot shows the correlation between the estimated coefficients  $\hat{\beta}_0$  and  $\hat{\beta}_1$ . On the left with 100 simulated straight lines, on the right with 10000.



c) The following results depend on the concrete simulation, unless you fix the randomized values with **set** . **seed()**:

```
1]))
## variation of beta_0 (100 simulations): 0.7193682
cat ("arithmetic mean of beta_0 (10000 simulations): ", mean (coef2[,
    1]))
## arithmetic mean of beta_0 (10000 simulations): 4.001601
cat ("standard deviation of beta_0 (10000 simulations): ",
    sd(coef2[, 1]))
## standard deviation of beta_0 (10000 simulations): 0.8627985
cat("variation of beta_0 (10000 simulations): ", var(coef2[,
    1]))
## variation of beta_0 (10000 simulations): 0.7444213
## beta 1
cat("arithmetic mean of beta_1 (100 simulations): ", mean(coef[,
    2]))
## arithmetic mean of beta_1 (100 simulations): 2.00391
cat ("standard deviation of beta 1 (100 simulations): ",
    sd(coef[, 2]))
## standard deviation of beta_1 (100 simulations): 0.07282633
cat("variation of beta_1 (100 simulations): ", var(coef[,
    2]))
## variation of beta_1 (100 simulations): 0.005303674
cat("arithmetic mean of beta_1 (10000 simulations): ", mean(coef2[,
    2]))
## arithmetic mean of beta_1 (10000 simulations): 1.999616
cat ("standard deviation of beta_1 (10000 simulations): ",
    sd(coef2[, 2]))
## standard deviation of beta_1 (10000 simulations): 0.07211866
cat("variation of beta_1 (10000 simulations): ", var(coef2[,
    2]))
## variation of beta 1 (10000 simulations): 0.005201102
```

According to theory the estimates should scatter around  $\beta_0 = 4$  and  $\beta_1 = 2$  (due to the standard deviation of the error term  $\sigma = \sqrt{2}$ ). For the (estimated) variance of  $\hat{\beta}_0$  and  $\hat{\beta}_1$  the following formulae need to be calculated:

```
## se(beta_0) :
SSx <- sum((x_sim - mean(x_sim))^2)

sqrt(2 * (1/10 + mean(x_sim)^2/SSx))

## [1] 0.8616496

## se(beta_1) :

sqrt(2/SSx)

## [1] 0.0722064</pre>
```

The theoretical standard errors  $se(\hat{\beta}_0) = 0.862$  and  $se(\hat{\beta}_1) = 0.0722$  that we computed above correspond to the average deviation of the parameter estimates  $\hat{\beta}_0$  and  $\hat{\beta}_1$  around the true parameter values  $\beta_0$  and  $\beta_1$ .

The more simulations we run, the closer the emprirical standard deviations of the set of estimates  $\hat{\beta}_0$  and  $\hat{\beta}_1$  get to the *true* standard deviations  $\operatorname{se}(\hat{\beta}_0)$  and  $\operatorname{se}(\hat{\beta}_1)$ . On the basis of 10 000 simulations we find  $\operatorname{se}(\hat{\beta}_0) \approx 0.8616496$  and  $\operatorname{se}(\hat{\beta}_1) \approx 0.0721$ . We conclude that the theoretical standard errors  $\operatorname{se}(\hat{\beta}_0)$  and  $\operatorname{se}(\hat{\beta}_1)$  and the (approximately) true values of  $\operatorname{se}(\hat{\beta}_0)$  and  $\operatorname{se}(\hat{\beta}_1)$  agree to a high degree.