

||| Chapter 6

Multiple Linear Regression (solutions to exercises)

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6.1 Nitrate concentration

|||| Exercise 6.1 Nitrate concentration

In order to analyze the effect of reducing nitrate loading in a Danish fjord, it was decided to formulate a linear model that describes the nitrate concentration in the fjord as a function of nitrate loading, it was further decided to correct for fresh water runoff. The resulting model was

$$Y_i = \beta_0 + \beta_1 x_{1,i} + \beta_2 x_{2,i} + \varepsilon_i, \quad \varepsilon_i \sim N(0, \sigma^2), \quad (6-1)$$

where Y_i is the natural logarithm of nitrate concentration, $x_{1,i}$ is the natural logarithm of nitrate loading, and $x_{2,i}$ is the natural logarithm of fresh water run off.

- a) Which of the following statements are assumed fulfilled in the usual multiple linear regression model?
- 1) $\varepsilon_i = 0$ for all $i = 1, \dots, n$, and β_j follows a normal distribution
 - 2) $E[x_1] = E[x_2] = 0$ and $V[\varepsilon_i] = \beta_1^2$
 - 3) $E[\varepsilon_i] = 0$ and $V[\varepsilon_i] = \beta_1^2$
 - 4) ε_i is normally distributed with constant variance, and ε_i and ε_j are independent for $i \neq j$
 - 5) $\varepsilon_i = 0$ for all $i = 1, \dots, n$, and x_j follows a normal distribution for $j = \{1, 2\}$

|||| Solution

- 1) ε_i follows a normal distribution with expectation equal zero, but the realizations are not zero, and further β_j is deterministic and hence it does not follow a distribution ($\hat{\beta}_j$ does), hence 1) is not correct
- 2)- 3) There are no assumptions on the expectation of x_j and the variance of ε equal σ^2 , not β_1^2 hence 2) and 3) are not correct
- 4) Is correct, this is the usual assumption about the errors
- 5) Is incorrect since ε_j follow a normal distribution, further there are no distributional assumptions on x_j . In fact we assume that x_j is known

The parameters in the model were estimated in R and the following results are available (slightly modified output from summary):

```
> summary(lm(y ~ x1 + x2))
```

Call:

```
lm(formula = y ~ x1 + x2)
```

Coefficients:

	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	-2.36500	0.22184	-10.661	< 2e-16
x1	0.47621	0.06169	7.720	3.25e-13
x2	0.08269	0.06977	1.185	0.237

Residual standard error: 0.3064 on 237 degrees of freedom

Multiple R-squared: 0.3438, Adjusted R-squared: 0.3382

F-statistic: 62.07 on 2 and 237 DF, p-value: < 2.2e-16

- b) What are the parameter estimates for the model parameters ($\hat{\beta}_i$ and $\hat{\sigma}^2$) and how many observations are included in the estimation?

||| Solution

The number of degrees of freedom is equal $n - (p + 1)$, and since the number of degrees of freedom is 237 and $p = 2$, we get $n = 237 + 2 + 1 = 240$. The parameters are given in the first column of the coefficient matrix, i.e.

$$\hat{\beta}_0 = -2.365 \quad (6-2)$$

$$\hat{\beta}_1 = 0.476 \quad (6-3)$$

$$\hat{\beta}_2 = 0.083 \quad (6-4)$$

and finally the estimated error variance is $\hat{\sigma}^2 = 0.3064^2$.

- c) Calculate the usual 95% confidence intervals for the parameters (β_0, β_1 , and β_2).

||| Solution

From Theorem 6.5 we know that the confidence intervals can be calculated by

$$\hat{\beta}_i \pm t_{1-\alpha/2} \hat{\sigma}_{\beta_i},$$

where $t_{1-\alpha/2}$ is based on 237 degrees of freedom, and with $\alpha = 0.05$, we get $t_{0.975} = 1.97$. The standard errors for the estimates is the second column of the coefficient matrix, and the confidence intervals become

$$\hat{\beta}_0 = -2.365 \pm 1.97 \cdot 0.222 \quad (6-5)$$

$$\hat{\beta}_1 = 0.467 \pm 1.97 \cdot 0.062 \quad (6-6)$$

$$\hat{\beta}_2 = 0.083 \pm 1.97 \cdot 0.070 \quad (6-7)$$

- d) On level $\alpha = 0.05$ which of the parameters are significantly different from 0, also find the p -values for the tests used for each of the parameters?

||| Solution

We can see directly from the confidence intervals above that β_0 and β_1 are significantly different from zero (the confidence intervals does not cover zero), while we cannot reject that $\beta_2 = 0$ (the confidence interval cover zero). The p -values we can see directly in the R output: for β_0 is less than 10^{-16} and the p -value for β_1 is $3.25 \cdot 10^{-13}$, i.e. very strong evidence against the null hypothesis in both cases.

6.2 Multiple linear regression model

|||| Exercise 6.2 Multiple linear regression model

The following measurements have been obtained in a study:

No.	1	2	3	4	5	6	7	8	9	10	11	12	13
y	1.45	1.93	0.81	0.61	1.55	0.95	0.45	1.14	0.74	0.98	1.41	0.81	0.89
x_1	0.58	0.86	0.29	0.20	0.56	0.28	0.08	0.41	0.22	0.35	0.59	0.22	0.26
x_2	0.71	0.13	0.79	0.20	0.56	0.92	0.01	0.60	0.70	0.73	0.13	0.96	0.27
No.	14	15	16	17	18	19	20	21	22	23	24	25	
y	0.68	1.39	1.53	0.91	1.49	1.38	1.73	1.11	1.68	0.66	0.69	1.98	
x_1	0.12	0.65	0.70	0.30	0.70	0.39	0.72	0.45	0.81	0.04	0.20	0.95	
x_2	0.21	0.88	0.30	0.15	0.09	0.17	0.25	0.30	0.32	0.82	0.98	0.00	

It is expected that the response variable y can be described by the independent variables x_1 and x_2 . This imply that the parameters of the following model should be estimated and tested

$$Y_i = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \varepsilon_i, \quad \varepsilon_i \sim N(0, \sigma^2).$$

- a) Calculate the parameter estimates ($\hat{\beta}_0$, $\hat{\beta}_1$, $\hat{\beta}_2$, and $\hat{\sigma}^2$), in addition find the usual 95% confidence intervals for β_0 , β_1 , and β_2 .

You can copy the following lines to R to load the data:

```
D <- data.frame(
  x1=c(0.58, 0.86, 0.29, 0.20, 0.56, 0.28, 0.08, 0.41, 0.22,
       0.35, 0.59, 0.22, 0.26, 0.12, 0.65, 0.70, 0.30, 0.70,
       0.39, 0.72, 0.45, 0.81, 0.04, 0.20, 0.95),
  x2=c(0.71, 0.13, 0.79, 0.20, 0.56, 0.92, 0.01, 0.60, 0.70,
       0.73, 0.13, 0.96, 0.27, 0.21, 0.88, 0.30, 0.15, 0.09,
       0.17, 0.25, 0.30, 0.32, 0.82, 0.98, 0.00),
  y=c(1.45, 1.93, 0.81, 0.61, 1.55, 0.95, 0.45, 1.14, 0.74,
       0.98, 1.41, 0.81, 0.89, 0.68, 1.39, 1.53, 0.91, 1.49,
       1.38, 1.73, 1.11, 1.68, 0.66, 0.69, 1.98)
)
```

||| Solution

The question is answered by R. Start by loading data into R and estimate the parameters in R

```
fit <- lm(y ~ x1 + x2, data=D)
summary(fit)
```

Call:

```
lm(formula = y ~ x1 + x2, data = D)
```

Residuals:

```
      Min       1Q   Median       3Q      Max
-0.155 -0.078 -0.020  0.050  0.301
```

Coefficients:

	Estimate	Std. Error	t value	Pr(> t)	
(Intercept)	0.43355	0.06598	6.57	1.3e-06	***
x1	1.65299	0.09525	17.36	2.5e-14	***
x2	0.00394	0.07485	0.05	0.96	

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.113 on 22 degrees of freedom

Multiple R-squared: 0.94, Adjusted R-squared: 0.934

F-statistic: 172 on 2 and 22 DF, p-value: 3.7e-14

||| Solution

The parameter estimates are given in the first column of the coefficient matrix, i.e.

$$\hat{\beta}_0 = 0.434,$$

$$\hat{\beta}_1 = 1.653,$$

$$\hat{\beta}_2 = 0.0039,$$

and the error variance estimate is $\hat{\sigma}^2 = 0.11^2$. The confidence intervals can either be calculated using the second column of the coefficient matrix, and the value of $t_{0.975}$ (with degrees of freedom equal 22), or directly in R:

```

confint(fit)

                2.5 % 97.5 %
(Intercept)  0.2967 0.5704
x1           1.4555 1.8505
x2          -0.1513 0.1592

```

b) Still using confidence level $\alpha = 0.05$ reduce the model if appropriate.

||| Solution

Since the confidence interval for β_2 cover zero (and the p -value is much larger than 0.05), the parameter should be removed from the model to get the simpler model

$$y_i = \beta_0 + \beta_1 x_1 + \varepsilon_i, \quad \varepsilon_i \sim N(0, \sigma^2),$$

the parameter estimates in the simpler model are

```

fit <- lm(y ~ x1, data=D)
summary(fit)

Call:
lm(formula = y ~ x1, data = D)

Residuals:
    Min       1Q   Median       3Q      Max
-0.1563 -0.0763 -0.0215  0.0516  0.2999

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  0.4361     0.0440   9.91 9.0e-10 ***
x1          1.6512     0.0871  18.96 1.5e-15 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.11 on 23 degrees of freedom
Multiple R-squared:  0.94, Adjusted R-squared:  0.937
F-statistic: 360 on 1 and 23 DF, p-value: 1.54e-15

```

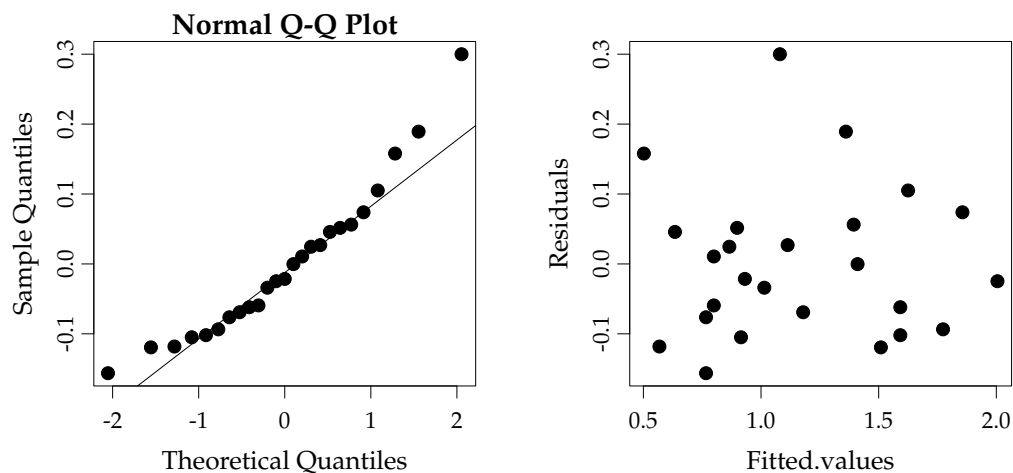
and both parameters are now significant.

- c) Carry out a residual analysis to check that the model assumptions are fulfilled.

||| Solution

We are interested in inspecting a q-q plot of the residuals and a plot of the residuals as a function of the fitted values

```
par(mfrow=c(1,2))
qqnorm(fit$residuals, pch=19)
qqline(fit$residuals)
plot(fit$fitted.values, fit$residuals, pch=19,
      xlab="Fitted.values", ylab="Residuals")
```

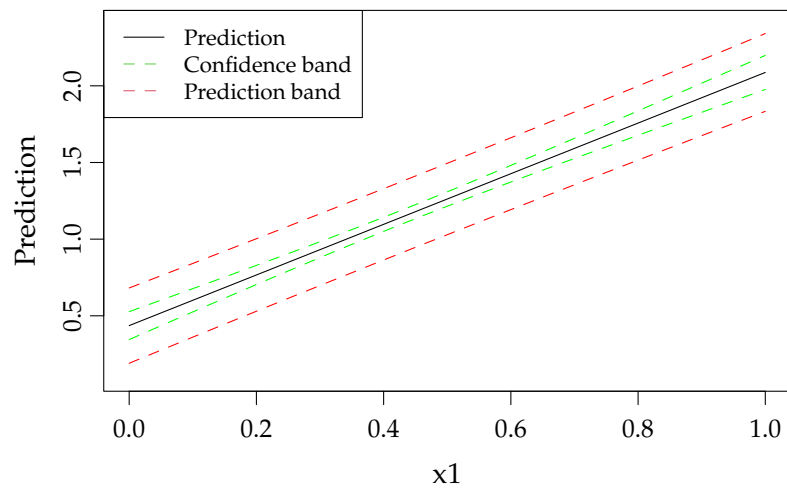


there are no strong evidence against the assumptions, the qq-plot is are a straight line and the are no obvious dependence between the residuals and the fitted values, and we conclude that the assumptions are fulfilled.

- d) Make a plot of the fitted line and 95% confidence and prediction intervals of the line for $x_1 \in [0, 1]$ (it is assumed that the model was reduced above).

||| Solution

```
x1new <- seq(0,1,by=0.01)
pred <- predict(fit, newdata=data.frame(x1=x1new),
               interval="prediction")
conf <- predict(fit, newdata=data.frame(x1=x1new),
               interval="confidence")
plot(x1new, pred[, "fit"], type="l", ylim=c(0.1,2.4),
     xlab="x1", ylab="Prediction")
lines(x1new, conf[, "lwr"], col="green", lty=2)
lines(x1new, conf[, "upr"], col="green", lty=2)
lines(x1new, pred[, "lwr"], col="red", lty=2)
lines(x1new, pred[, "upr"], col="red", lty=2)
legend("topleft", c("Prediction", "Confidence band", "Prediction band"),
      lty=c(1,2,2), col=c(1,3,2), cex=0.7)
```



6.3 MLR simulation exercise

|||| Exercise 6.3 MLR simulation exercise

The following measurements have been obtained in a study:

Nr.	1	2	3	4	5	6	7	8
y	9.29	12.67	12.42	0.38	20.77	9.52	2.38	7.46
x_1	1.00	2.00	3.00	4.00	5.00	6.00	7.00	8.00
x_2	4.00	12.00	16.00	8.00	32.00	24.00	20.00	28.00

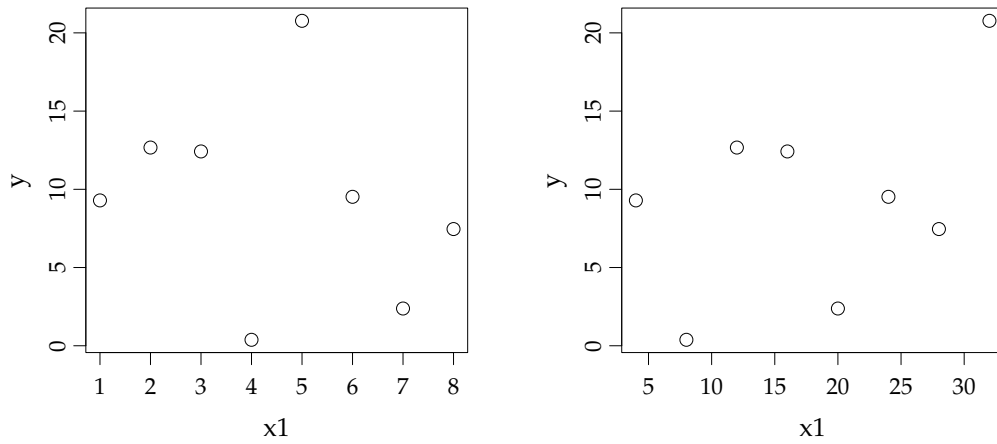
- a) Plot the observed values of y as a function of x_1 and x_2 . Does it seem reasonable that either x_1 or x_2 can describe the variation in y ?
You may copy the following lines into R to load the data

```
D <- data.frame(  
  y=c(9.29,12.67,12.42,0.38,20.77,9.52,2.38,7.46),  
  x1=c(1.00,2.00,3.00,4.00,5.00,6.00,7.00,8.00),  
  x2=c(4.00,12.00,16.00,8.00,32.00,24.00,20.00,28.00)  
)
```

|||| Solution

The data is plotted with

```
par(mfrow=c(1,2))  
plot(D$x1, D$y, xlab="x1", ylab="y")  
plot(D$x2, D$y, xlab="x1", ylab="y")
```



There does not seem to be a strong relation between y and x_1 or x_2 .

b) Estimate the parameters for the two models

$$Y_i = \beta_0 + \beta_1 x_{1,i} + \varepsilon_i, \quad \varepsilon_i \sim N(0, \sigma^2),$$

and

$$Y_i = \beta_0 + \beta_1 x_{2,i} + \varepsilon_i, \quad \varepsilon_i \sim N(0, \sigma^2),$$

and report the 95% confidence intervals for the parameters. Are any of the parameters significantly different from zero on a 5% confidence level?

||| Solution

The models are fitted with

```
fit1 <- lm(y ~ x1, data=D)
fit2 <- lm(y ~ x2, data=D)
confint(fit1)

                2.5 % 97.5 %
(Intercept) -0.5426 24.898
x1           -3.1448  1.893

confint(fit2)

                2.5 % 97.5 %
(Intercept) -7.5581 15.9659
x2           -0.2958  0.8688
```

since all confidence intervals cover zero we cannot reject that the parameters are in fact zero, and we would conclude neither x_1 nor x_2 explain the variations in y .

c) Estimate the parameters for the model

$$Y_i = \beta_0 + \beta_1 x_{1,i} + \beta_2 x_{2,i} + \varepsilon_i, \quad \varepsilon_i \sim (N(0, \sigma^2)), \quad (6-8)$$

and go through the steps of Method 6.16 (use confidence level 0.05 in all tests).

||| Solution

The model is fitted with

```
fit <- lm(y ~ x1 + x2, data=D)
summary(fit)
```

Call:

```
lm(formula = y ~ x1 + x2, data = D)
```

Residuals:

```
      1      2      3      4      5      6      7      8
0.9622 0.1783 -0.3670 -1.0963 -0.3448 -0.2842 0.0178 0.9339
```

Coefficients:

	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	8.0325	0.6728	11.9	0.0000727 ***
x1	-3.5734	0.1955	-18.3	0.0000090 ***
x2	0.9672	0.0489	19.8	0.0000061 ***

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.821 on 5 degrees of freedom

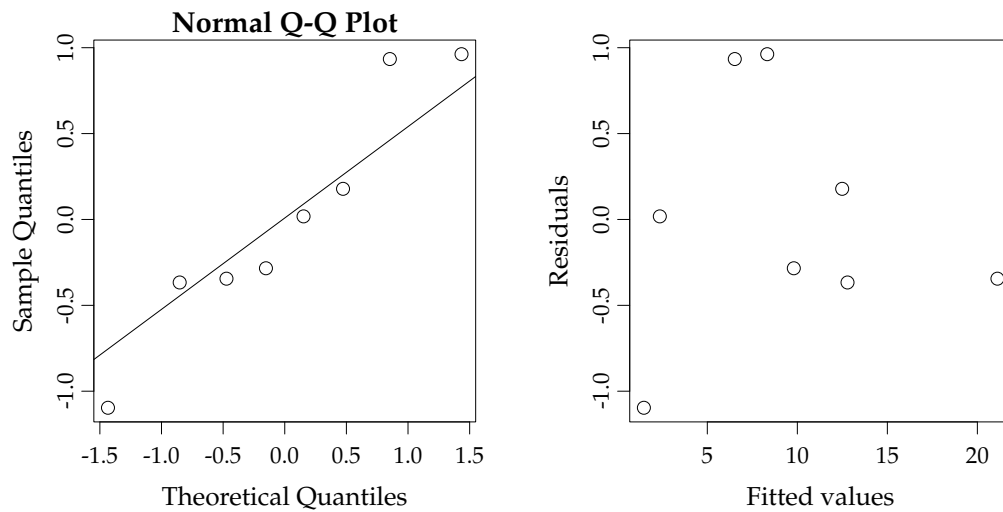
Multiple R-squared: 0.988, Adjusted R-squared: 0.983

F-statistic: 208 on 2 and 5 DF, p-value: 0.0000154

||| Solution

Before discussing the parameter let's have a look at the residuals:

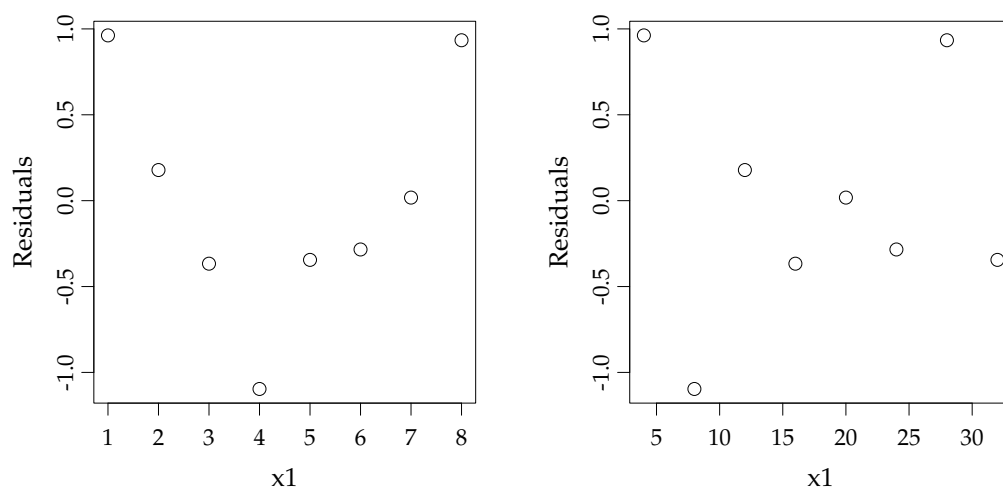
```
par(mfrow=c(1,2))
qqnorm(fit$residuals)
qqline(fit$residuals)
plot(fit$fitted.values, fit$residuals,
      xlab="Fitted values", ylab="Residuals")
```



There are no obvious structures in the residuals as a function of the fitted values and also there does not seem to be a serious departure from normality, but let's try to look at the residuals as a function of the independent variables anyway.

||| Solution

```
par(mfrow=c(1,2))
plot(D$x1, fit$residuals, xlab="x1", ylab="Residuals")
plot(D$x2, fit$residuals, xlab="x1", ylab="Residuals")
```



The plot of the residuals as a function of x_1 suggests that there could be a quadratic dependence.

||| Solution

Now include the quadratic dependence of x_1

```
D$x3 <- D$x1^2
fit3 <- lm(y ~ x1 + x2 + x3, data=D)
summary(fit3)
```

Call:
lm(formula = y ~ x1 + x2 + x3, data = D)

Residuals:

	1	2	3	4	5	6	7	8
	0.0417	-0.0233	-0.0107	-0.0754	-0.0252	0.1104	0.0585	-0.0758

Coefficients:

	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	10.1007	0.1212	83.3	1.2e-07 ***
x1	-5.0024	0.0709	-70.5	2.4e-07 ***
x2	1.0006	0.0054	185.2	5.1e-09 ***
x3	0.1474	0.0070	21.1	3.0e-05 ***

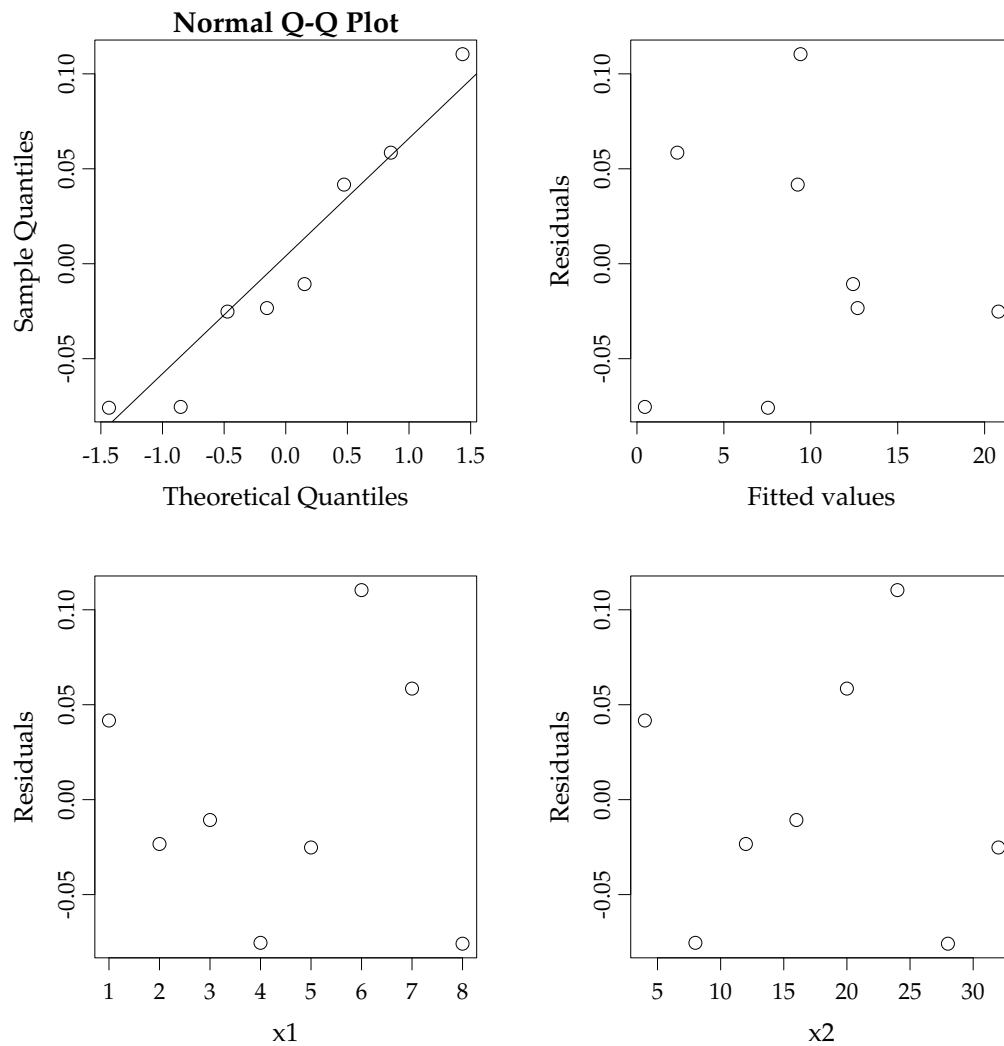
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.0867 on 4 degrees of freedom
Multiple R-squared: 1, Adjusted R-squared: 1
F-statistic: 1.26e+04 on 3 and 4 DF, p-value: 2.11e-08

we can see that all parameters are still significant, and we can do the residual analysis of the resulting model.

||| Solution

```
par(mfrow=c(2,2))
qqnorm(fit3$residuals)
qqline(fit3$residuals)
plot(fitted.values(fit3), fit3$residuals,
      xlab="Fitted values", ylab="Residuals")
plot(D$x1, fit3$residuals, xlab="x1", ylab="Residuals")
plot(D$x2, fit3$residuals, xlab="x2", ylab="Residuals")
```

There are no obvious structures left and there is no departure from normality, and we can report the finally selected model as

$$Y_i = \beta_0 + \beta_1 x_{1,i} + \beta_2 x_{2,i} + \beta_3 x_{1,i}^2 + \varepsilon_i, \quad \varepsilon_i \sim (N(0, \sigma^2)),$$

with the parameters estimates given above.

- d) Find the standard error for the line, and the confidence and prediction intervals for the line for the points $(\min(x_1), \min(x_2))$, (\bar{x}_1, \bar{x}_2) , $(\max(x_1), \max(x_2))$.

||| Solution

The question is solved by

```
## New data
Dnew <- data.frame(x1=c(min(D$x1),mean(D$x1),max(D$x1)),
                  x2=c(min(D$x2),mean(D$x2),max(D$x2)),
                  x3=c(min(D$x1),mean(D$x1),max(D$x1))^2)

## standard error for the line
predict(fit3, newdata=Dnew, se=TRUE)$se

      1      2      3
0.07306 0.04785 0.07985

## Confidence interval
predict(fit3, newdata=Dnew, interval="confidence")

      fit    lwr    upr
1  9.248  9.045  9.451
2  8.587  8.454  8.720
3 11.538 11.317 11.760

## Prediction interval
predict(fit3, newdata=Dnew, interval="prediction")

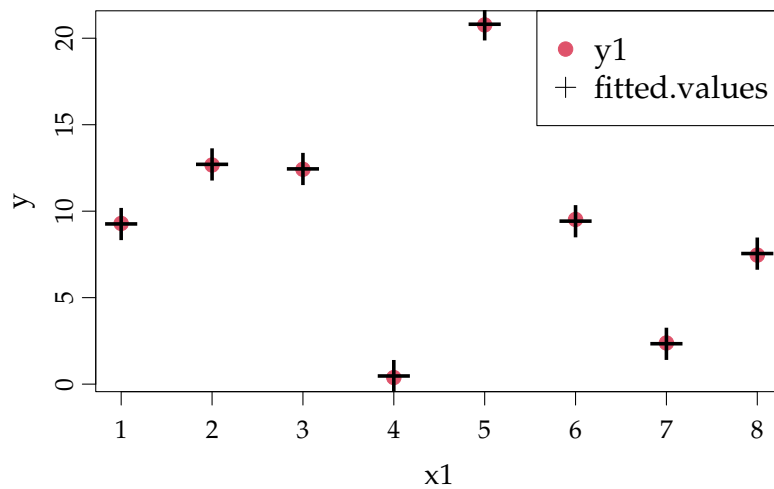
      fit    lwr    upr
1  9.248  8.934  9.563
2  8.587  8.312  8.862
3 11.538 11.211 11.866
```

- e) Plot the observed values together with the fitted values (e.g. as a function of x_1).

||| Solution

The question is solved by

```
plot(D$x1, D$y, pch=19, col=2, xlab="x1", ylab="y")
points(D$x1, fit3$fitted.values, pch="+", cex=2)
legend("topright", c("y1", "fitted.values"), pch=c(19,3), col=c(2,1))
```



Notice that we have an almost perfect fit when including x_1 , x_2 and x_1^2 in the model, while neither x_1 nor x_2 alone could predict the outcomes.