STAT 210
Applied Statistics and Data Analysis
Week 9 - Summary

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V29: Linear Regression 3
Confidence Bands and Anova

Confidence Bands for the Regression Line

Confidence Bands for the Regression Line

Notation: $\mu_{Y|x} = \mathsf{E}(Y|X = x)$

Recall that

$$E(Y|X) = \beta_0 + \beta_1 X$$

For $\mu_{Y|x}$, there are two sources of variability, $\hat{\beta}_0$, and $\hat{\beta}_1$.

The standard error (or empirical standard deviation) of $\mu_{Y|x}$ is

$$se_{\mu_{Y|x}} = \hat{\sigma}\Big(\frac{1}{n} + \frac{(x - \bar{x})^2}{\sum_i (x_i - \bar{x})^2}\Big)^{1/2}. \tag{1}$$

Observe that the standard error is a minimum when $x = \bar{x}$.

Confidence Band for the Regression Line

A confidence interval for the average value of Y at x at the $(1-\alpha)$ level is given by

$$\left(\hat{\beta}_0 + \hat{\beta}_1 x - t_{n-2,1-\alpha/2} se_{\mu_{Y|x}}, \hat{\beta}_0 + \hat{\beta}_1 x + t_{n-2,1-\alpha/2} se_{\mu_{Y|x}}\right)$$

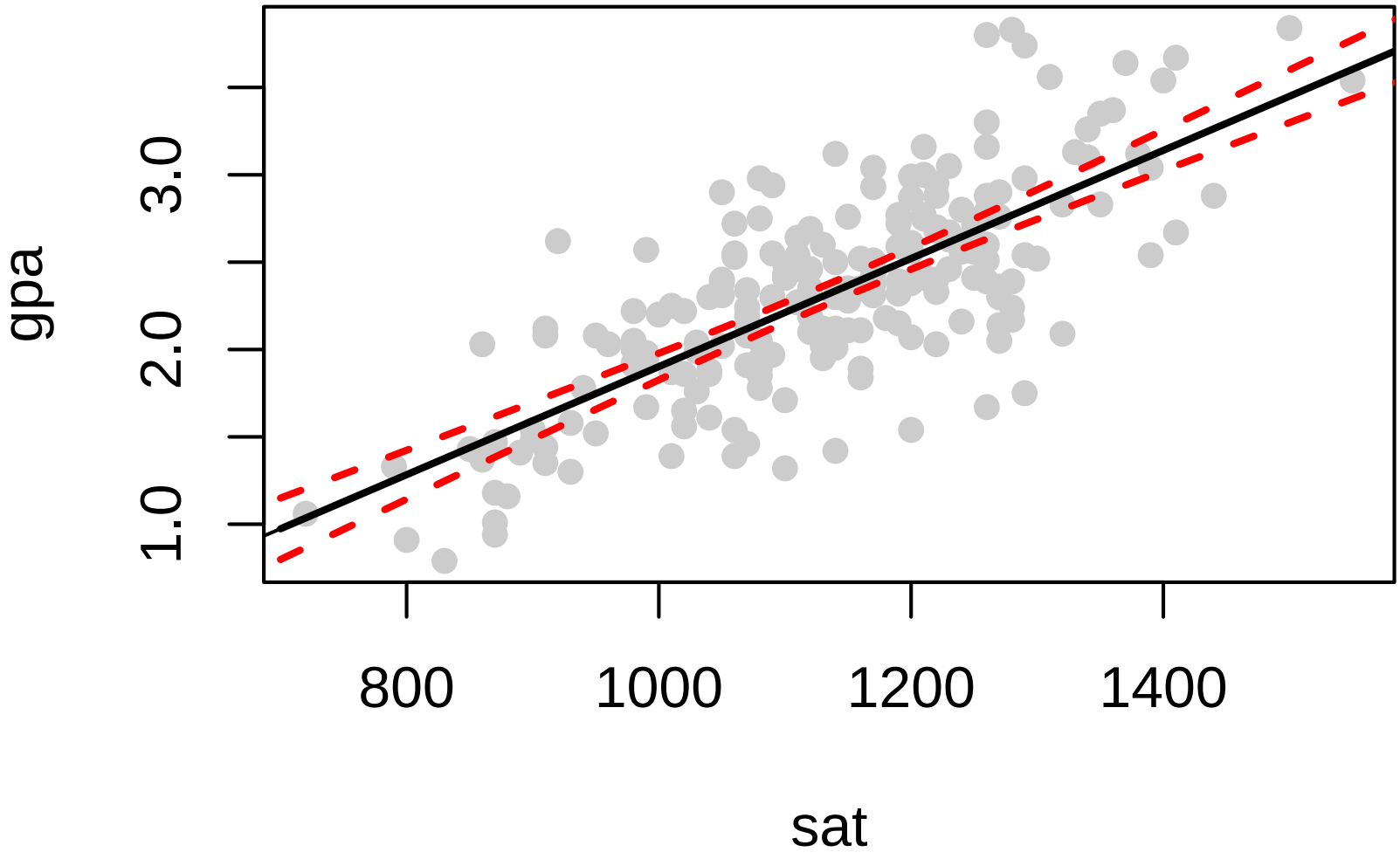
We can get these intervals using the function `predict`, which, when applied to an object of class `lm` and a data frame of x values, will give the values of the regression line at the x values, with the option of adding confidence intervals.

```
new.data <- data.frame(x=c(900,1100,1300))
predict(model,new.data,interval='c')
```

```
##        fit      lwr      upr
## 1 1.592779 1.486950 1.698609
## 2 2.211634 2.154371 2.268896
## 3 2.830488 2.746088 2.914887
```

Confidence Band for the Regression Line

Let us use this to draw 'confidence bands' for the regression line in this example.



Confidence Band for the Regression Line

```
plot(sat, gpa)
modelA <- lm(gpa~sat, data = Grades)
abline(modelA)
new.sat <- data.frame(sat=seq(700,1600,
                              length.out = 15))
pc <- predict(modelA,new.sat, int='c')
matlines(new.sat$sat, pc, lty=c(1,2,2),
         lwd=rep(2,3),
         col=c('black','red','red'))
```

Confidence Band for the Regression Line

If we wanted to predict the value of y corresponding to a given value of x (instead of predicting the *average* value of y at x), we would expect a wider confidence band.

To avoid confusion, these are called **prediction** intervals.

Prediction intervals are wider because they take into account sampling variability due to the error term in the model.

Also, since the uncertainty in the estimation of the parameters is less important, their curvature is less pronounced.

The standard error for the predicted value $\hat{y}$ at the point x is given by

$$se_{\hat{y}|x} = \hat{\sigma}\left(1 + \frac{1}{n} + \frac{(x - \bar{x})^2}{\sum_i (x_i - \bar{x})^2}\right)^{1/2}.$$

Confidence Band for the Regression Line

A prediction interval for the value $\hat{y}$ at the point x and the $(1-\alpha)$ level is given by

$$\left(\hat{\beta}_0 + \hat{\beta}_1 x - t_{n-2,1-\alpha/2} se_{\hat{y}|x}, \hat{\beta}_0 + \hat{\beta}_1 x + t_{n-2,1-\alpha/2} se_{\hat{y}|x}\right)$$

The `predict` function also calculates prediction intervals.

```
new.data <- data.frame(x=c(900,1100,1300))
predict(model,new.data,interval='p')
```

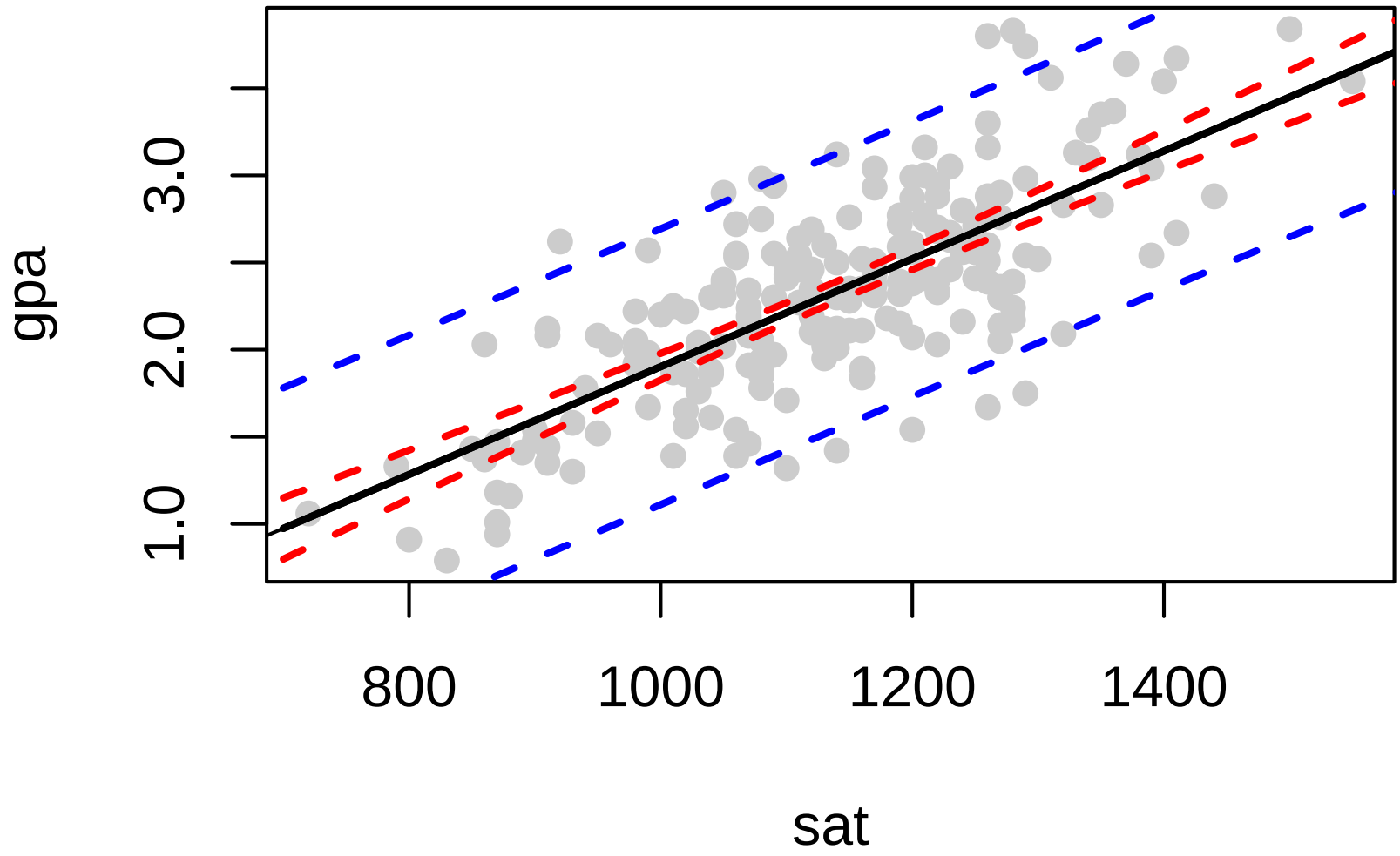
```
##        fit       lwr      upr
## 1 1.592779 0.7979927 2.387566
## 2 2.211634 1.4218455 3.001422
## 3 2.830488 2.0382696 3.622706
```

```
predict(model,new.data,interval='c')
```

```
##        fit      lwr      upr
## 1 1.592779 1.486950 1.698609
## 2 2.211634 2.154371 2.268896
## 3 2.830488 2.746088 2.914887
```

Confidence Band for the Regression Line

Let's now draw a graph including both bands for comparison.



Confidence Band for the Regression Line

```
plot(sat, gpa)
modelA <- lm(gpa~sat, data = Grades)
abline(modelA)
new.sat <- data.frame(sat=seq(700,1600,
                              length.out = 15))
pc <- predict(modelA,new.sat, int='c')
matlines(new.sat$sat, pc, lty=c(1,2,2),lwd=rep(2,3),
         col=c('black','red','red'))
pp <- predict(modelA,new.sat, int='p')
matlines(new.sat$sat, pp, lty=c(1,2,2),lwd=rep(2,3),
         col=c('black','red','red'))
```

Analysis of Variance in Linear Regression

Analysis of Variance in Linear Regression

Anova is based on dividing the sums of squares and degrees of freedom associated with the response variable Y.

The difference $y_i - \bar{y}$ is divided into two parts:

1.- The deviation of y_i from the regression line: $y_i - \hat{y}_i$.

2.- The deviation of the fitted value $\hat{y}_i$ from the mean: $\hat{y}_i - \bar{y}$.

$$y_i - \bar{y} = y_i - \hat{y}_i + \hat{y}_i - \bar{y}$$

Squaring this relation and summing up over i we get

$$\begin{aligned} \sum_{i=1}^{n}(y_i - \bar{y})^2 &= \sum_{i=1}^{n}(y_i - \hat{y}_i + \hat{y}_i - \bar{y})^2 \\ &= \sum_{i=1}^{n}(y_i - \hat{y}_i)^2 + \sum_{i=1}^{n}(\hat{y}_i - \bar{y})^2 \end{aligned} \tag{2}$$

This relation is commonly expressed as

$$SST = SSE + SSR$$

where

- SST denotes the total sum of squares,
- SSE is the error or residual sum of squares and
- SSR is the regression sum of squares.

The terms $y_i - \bar{y}$ represent the distance from the observed values to the average, $y_i - \hat{y}_i$ is the distance between the observed and the fitted value and $\hat{y}_i - \bar{y}$ is the distance between the fitted value and the average observed value.

The degrees of freedom are similarly distributed.

There are $n-1$ degrees of freedom associated with SST; one degree is lost since we need to estimate the population mean μ by $\bar{y}$.

These degrees of freedom are divided into SSR and SSE.

The latter has $n-2$ degrees of freedom; two are lost because we need to calculate parameters β_0 and β_1, to fit the regression line.

Finally, there are two degrees of freedom associated with the regression line, one for the slope and one for the intercept, but one is lost since $\sum_i(\hat{y}_i - \bar{y}) = 0$ by property 1, so that SSR has one degree of freedom.

Sums of squares divided by their degrees of freedom are known as **mean squares** and are denoted by MS, thus

$$MSE = \frac{SSE}{n-2}, \qquad \text{and} \qquad MSR = \frac{SSR}{1} = SSR.$$

We have assumed that the errors in the regression are centered normal with variance σ^2, and therefore $SSE/\sigma^2 \sim \chi^2_{n-2}$, this gives $E(SSE/\sigma^2) = n-2$ and

$$E(MSE) = E\Big(\frac{SSE}{n-2}\Big) = \sigma^2,$$

which means that MSE is an unbiased estimator of σ^2.

$$
\begin{aligned}
E(MSR) &= E(\hat{\beta}_1^2) \sum_{i=1}^{n} (x_i - \bar{x})^2 \\
&= \left(Var(\hat{\beta}_1) + \left(E(\hat{\beta}_1) \right)^2 \right) \sum_{i=1}^{n} (x_i - \bar{x})^2 \\
&= \sigma^2 + \beta_1^2 \sum_{i=1}^{n} (x_i - \bar{x})^2.
\end{aligned}
$$

When $\beta_1 = 0$, the mean of the sampling distribution of MSR is σ^2 and coincides with the mean of MSE.

If $\beta_1 = 0$, the quantities SSR/σ^2 and SSE/σ^2 have a χ^2 distribution with 1 and $n - 2$ degrees of freedom, and it is possible to show that they are independent.

In consequence,

$$\frac{MSR}{MSE} = \frac{\frac{SSR/\sigma^2}{1}}{\frac{SSE/\sigma^2}{n-2}} = \frac{\chi^2_1/1}{\chi^2_{n-2}/(n-2)} \sim F_{1,n-2}.$$

Therefore, to test $H_0 : \beta_1 = 0$ we use this statistic. If msR and msE are the observed values for the sums of squares then

$$F_{obs} = \frac{msR}{msE}$$

and large values of F_{obs} give evidence against the null hypothesis.

At a confidence level of $1 - \alpha$, the null hypothesis will be rejected if

$$F_{obs} \geq F_{1,n-2,1-\alpha}.$$

Analysis of Variance in Linear Regression

The usual way to sum up these results is through an Analysis of Variance (Anova) table.

Table 1: Anova table for example 1.

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Squares	F_{obs}	Critical F
Regression	SSR	1	$MSR = \frac{SSR}{1}$	$F = \frac{MSR}{MSE}$	`qf(1-`α`, 1, n-2)`
Error	SSE	$n-2$	$MSE = \frac{SSE}{n-2}$		
Total	SST	$n-1$			

Analysis of Variance in Linear Regression

In R we get an anova table with the command anova acting on an object of class lm:

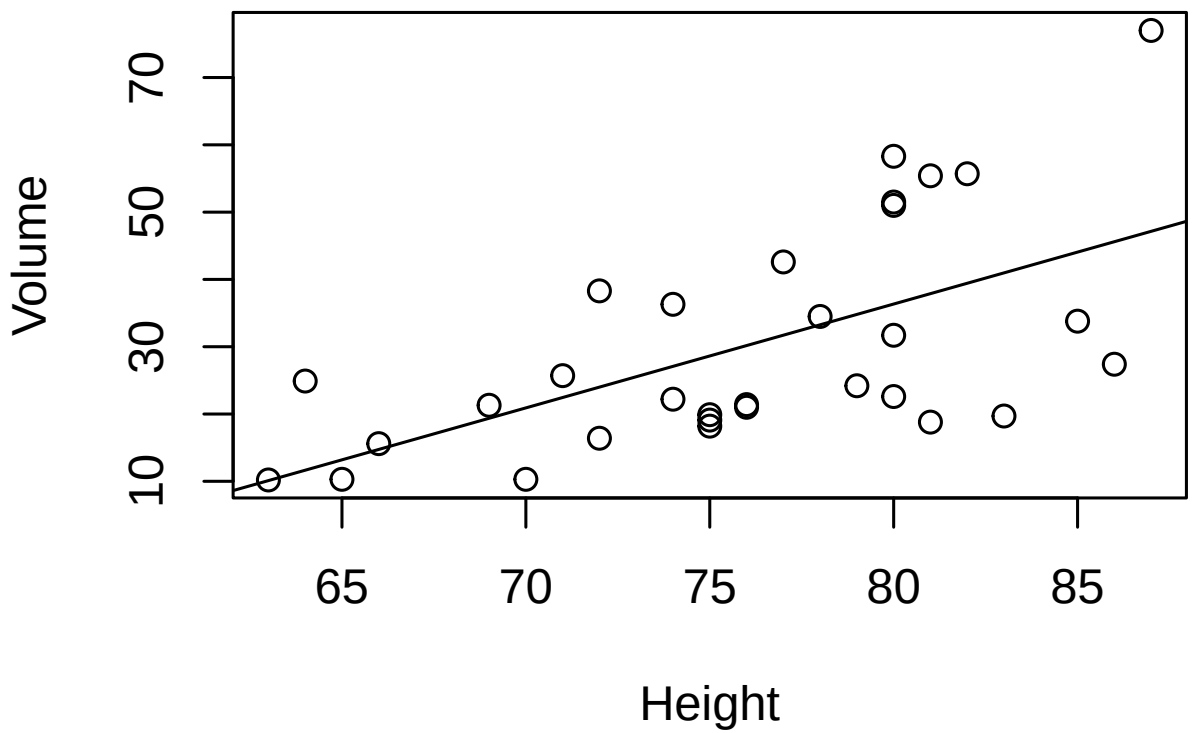
```
anova(lm1)
```

```
## Analysis of Variance Table
##
## Response: FL
##            Df  Sum Sq Mean Sq F value    Pr(>F)
## CL          1 2329.45 2329.45  4531.1 < 2.2e-16 ***
## Residuals 198  101.79    0.51
## ---
## Signif. codes:
## 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Example 3

The data set `trees` has data on girth, height, and volume of timber in 31 felled black cherry trees. Girth is the diameter of the tree in inches measured at 4 ft 6 in above the ground.

```
plot(Volume ~ Height, data=trees)
lm4 <- lm(Volume ~ Height, data=trees)
abline(lm4)
```



Example 3

```
summary(lm4)
```

```
##
## Call:
## lm(formula = Volume ~ Height, data = trees)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -21.274  -9.894  -2.894  12.068  29.852
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept) -87.1236    29.2731  -2.976 0.005835 **
## Height        1.5433     0.3839   4.021 0.000378 ***
## ---
## Signif. codes:
## 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 13.4 on 29 degrees of freedom
## Multiple R-squared:  0.3579, Adjusted R-squared:  0.3358
## F-statistic: 16.16 on 1 and 29 DF,  p-value: 0.0003784
```

```
anova(lm4)
```

```
## Analysis of Variance Table
##
## Response: Volume
##           Df Sum Sq Mean Sq F value    Pr(>F)
## Height     1 2901.2 2901.19  16.165 0.0003784 ***
## Residuals 29 5204.9  179.48
## ---
## Signif. codes:
## 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

V30: Simple Linear Regression 4: Coefficient of Determination

Coefficient of Determination

The analysis of variance is based on the following decomposition for the sum of squares:

$$SST = SSE + SSR.$$

Since the sums are non-negative we have that $SSE \leq SST$.

Observe that they are equal only if there is no relation between the two variables: $SSR = 0$ means that $\hat{y}_i = \bar{y}$ for all i and for this to be true, the regression line must be horizontal, so $\beta_1 = 0$ and $y = \beta_0$.

The regression sum of squares SSR is usually interpreted as the amount of variability in Y that is explained by the regression line.

The ratio SSE/SST represents the proportion of the variability that cannot be explained by the linear regression model.

The **coefficient of determination** R^2 is defined as

$$R^2 = 1 - \frac{SSE}{SST} = \frac{SSR}{SST} = \frac{\sum_{i=1}^{n}(\hat{y}_i - \bar{y})^2}{\sum_{i=1}^{n}(y_i - \bar{y})^2} \tag{3}$$

and represents the proportion of the variation that is explained by the regression model.

Recall the summary for the regression in the first example:

```
summary(lm1)
```

```
##
## Call:
## lm(formula = FL ~ CL)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -1.86395 -0.51746 -0.02826  0.50456  1.77009
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)  0.15316    0.23477   0.652    0.515
## CL           0.48060    0.00714  67.313   <2e-16 ***
## ---
## Signif. codes:
## 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.717 on 198 degrees of freedom
## Multiple R-squared:  0.9581, Adjusted R-squared:  0.9579
## F-statistic:  4531 on 1 and 198 DF,  p-value: < 2.2e-16
```

Coefficient of Determination

Although the model looks very good, we also fitted separate models for each species, which are `lm2` and `lm3`.

```
summary(lm2)
```

```
##
## Call:
## lm(formula = FL[sp == "B"] ~ CL[sp == "B"], data = crabs)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -0.95680 -0.17686 -0.01135  0.22143  0.82572
##
## Coefficients:
##                Estimate Std. Error t value Pr(>|t|)
## (Intercept)   0.971315   0.134562   7.218 1.13e-10 ***
## CL[sp == "B"] 0.435315   0.004364  99.745  < 2e-16 ***
## ---
## Signif. codes:
## 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.2997 on 98 degrees of freedom
## Multiple R-squared:  0.9902, Adjusted R-squared:  0.9901
## F-statistic:  9949 on 1 and 98 DF,  p-value: < 2.2e-16
```

Coefficient of Determination

```
summary(lm3)
```

```
##
## Call:
## lm(formula = FL[sp == "O"] ~ CL[sp == "O"], data = crabs)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -1.1344 -0.3357 -0.0249  0.2734  1.2282
##
## Coefficients:
##                Estimate Std. Error t value Pr(>|t|)
## (Intercept)   0.762041   0.257726   2.957   0.0039 **
## CL[sp == "O"] 0.478668   0.007404  64.651   <2e-16 ***
## ---
## Signif. codes:
## 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.4983 on 98 degrees of freedom
## Multiple R-squared:  0.9771, Adjusted R-squared:  0.9769
## F-statistic:  4180 on 1 and 98 DF,  p-value: < 2.2e-16
```

We see that the separate models are even better, accounting for 97.7 and 99% of the variability in the responses.

Coefficient of Determination

Let's look at the other two examples we have considered.

```
summary(lm4)
```

```
##
## Call:
## lm(formula = Volume ~ Height, data = trees)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -21.274  -9.894  -2.894  12.068  29.852
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept) -87.1236    29.2731  -2.976 0.005835 **
## Height        1.5433     0.3839   4.021 0.000378 ***
## ---
## Signif. codes:
## 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 13.4 on 29 degrees of freedom
## Multiple R-squared:  0.3579, Adjusted R-squared:  0.3358
## F-statistic: 16.16 on 1 and 29 DF,  p-value: 0.0003784
```

Coefficient of Determination

```
summary(lm5)
```

```
##
## 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 first of these models has a low R^2 of 35.8% while the second has a much better value of 93.5%.

Relation with the Correlation Coefficient

We have the following proposition:

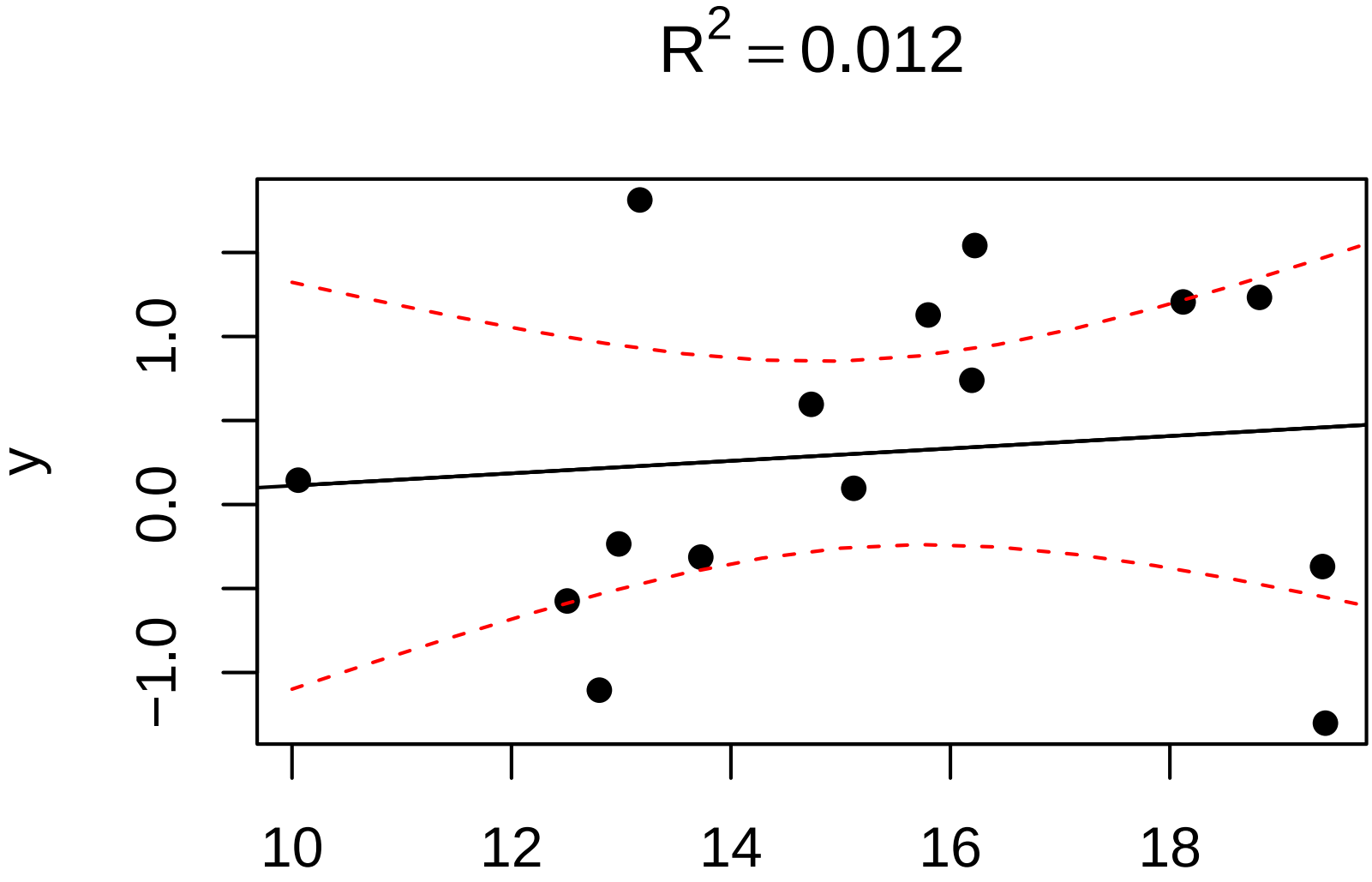
Proposition 1 Let ρ be the correlation coefficient for the sample $(x_i, y_i), i = 1, \ldots, n$. Then

$$R^2 = \rho^2.$$

It is important to observe that this relation is only true for simple regression. It does not hold in the multivariate case.

As an example let us look at some simulated data. First we look at purely random values.

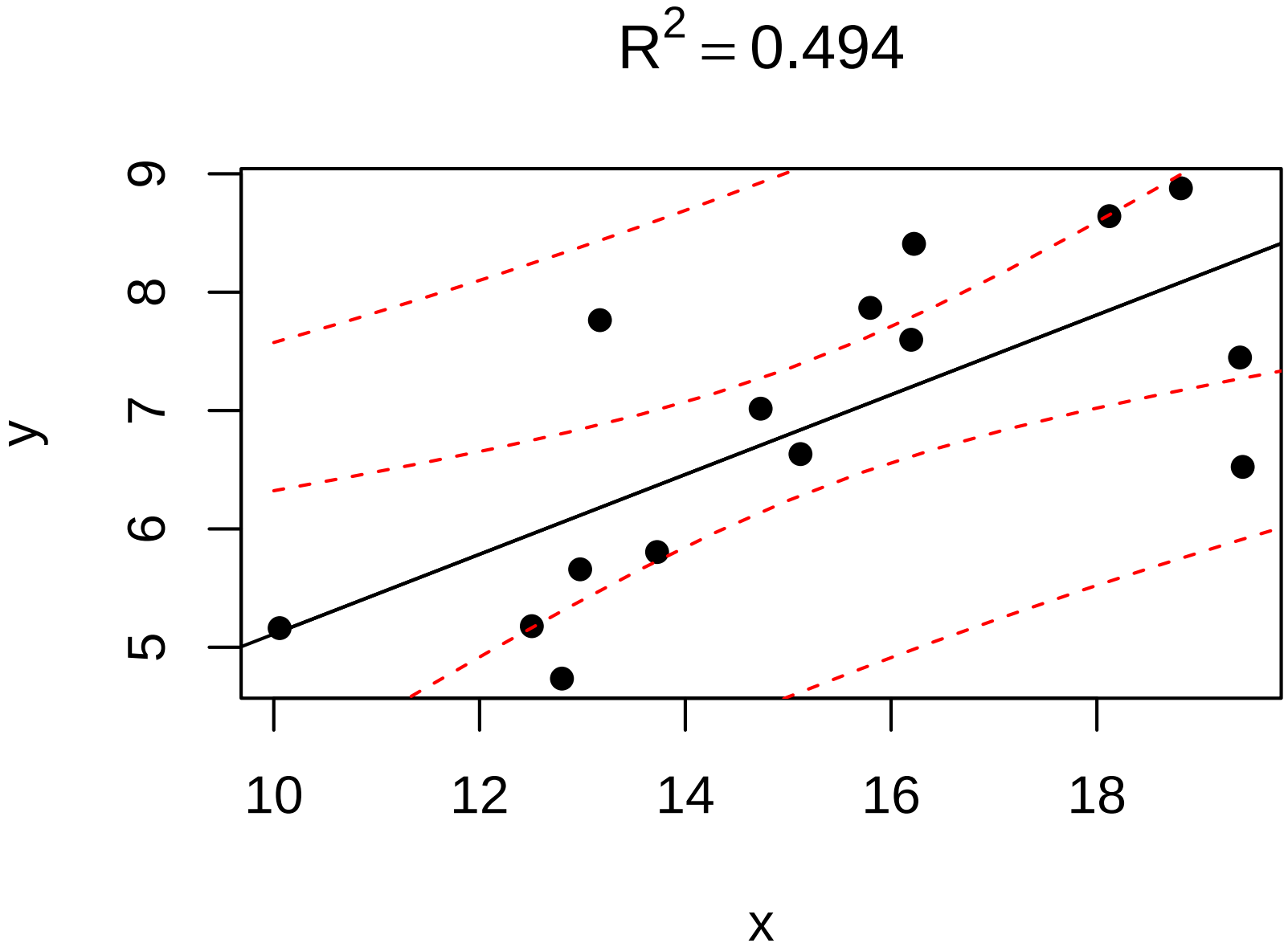
```
## [1] 0.012
```



Coefficient of Determination

```
set.seed(98765)
xx <- runif(15,10,20)
zz <- rnorm(15)
(r.sq <-round(summary(lm(zz~xx))$r.squared,3))
plot(xx,zz,pch=16, xlab='x', ylab='y')
abline(lm(zz~xx))
title(main= bquote(R^2 == .(r.sq)))
xx.new <- data.frame(xx=seq(10,20, length.out = 15))
pc <- predict(lm(zz~xx),xx.new, int='c')
matlines(xx.new$xx, pc, lty=c(1,2,2),
         col=c('black','red','red'))
pp <- predict(lm(zz~xx),xx.new, int='p')
matlines(xx.new$xx, pp, lty=c(1,2,2),
         col=c('black','red','red'))
```

```
## [1] 0.494
```

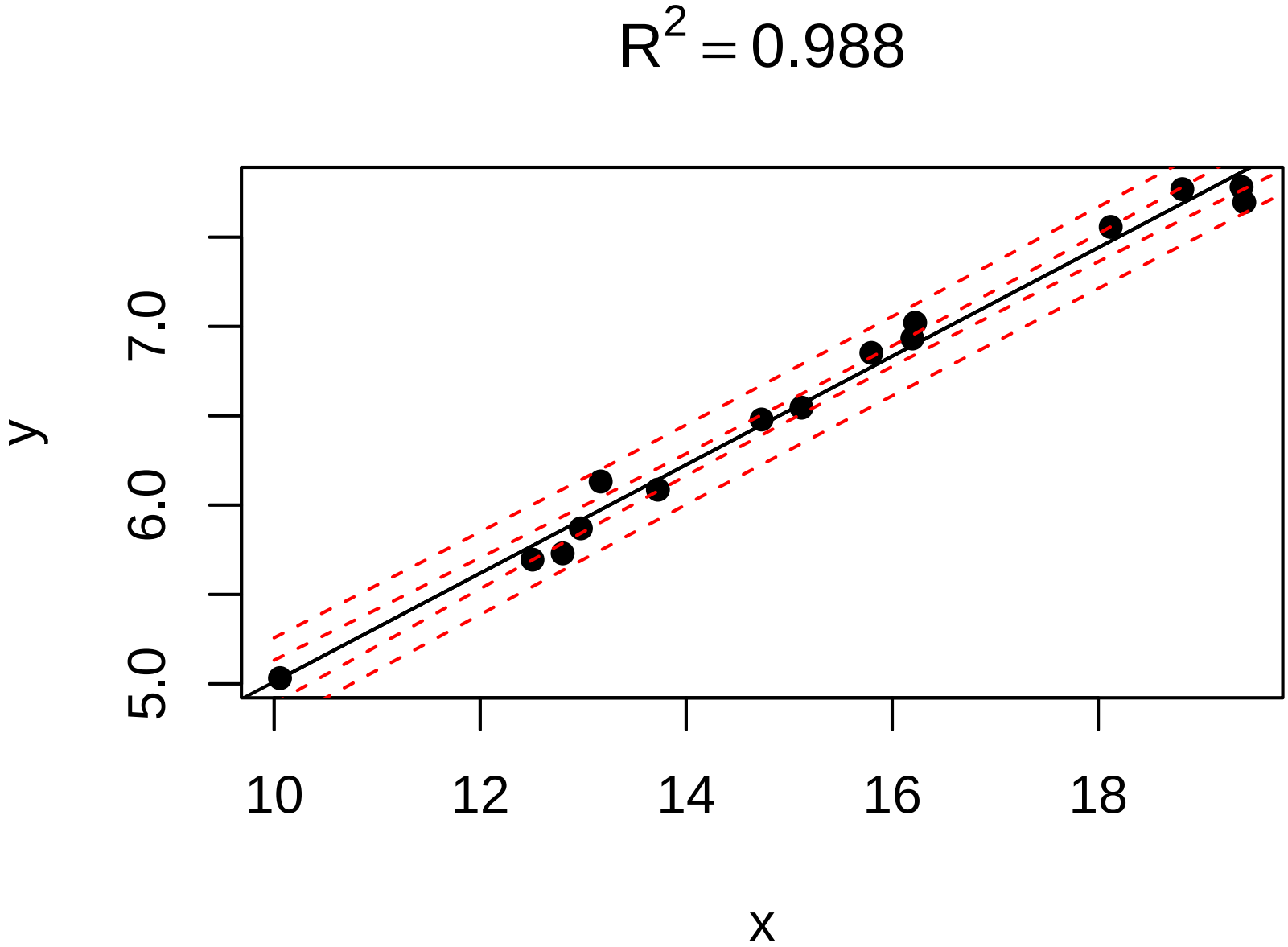


```
yy1 <- 2 + 0.3*xx + zz
plot(xx,yy1,pch=16, xlab='x', ylab='y')
abline(lm(yy1~xx))
(r.sq <-round(summary(lm(yy1~xx))$r.squared,3))
title(main= bquote(R^2 == .(r.sq)))
pc <- predict(lm(yy1~xx),xx.new, int='c')
matlines(xx.new$xx, pc, lty=c(1,2,2),
         col=c('black','red','red'))
pp <- predict(lm(yy1~xx),xx.new, int='p')
matlines(xx.new$xx, pp, lty=c(1,2,2),
         col=c('black','red','red'))
```

Now there is a linear relation between y and x but the variability due to the variance of the noise makes the explained variability to be only about 50%. As a third and final example, let us reduce noise variability by rescaling it.

```
yy2 <- 2 + 0.3*xx + zz/10
plot(xx,yy2,pch=16, xlab='x', ylab='y')
abline(lm(yy2~xx))
(r.sq <-round(summary(lm(yy2~xx))$r.squared,3))
title(main= bquote(R^2 == .(r.sq)))
pc <- predict(lm(yy2~xx),xx.new, int='c')
matlines(xx.new$xx, pc, lty=c(1,2,2),
         col=c('black','red','red'))
pp <- predict(lm(yy2~xx),xx.new, int='p')
matlines(xx.new$xx, pp, lty=c(1,2,2),
         col=c('black','red','red'))
```

```
## [1] 0.988
```



V 31: Simple Linear Regression 5: Model Assessment

The quality of a model depends on the veracity of the assumptions we have made, which are the basis for the estimation of the parameters.

We need to check the goodness-of-fit of the model and the possible presence of outliers or highly influential data points.

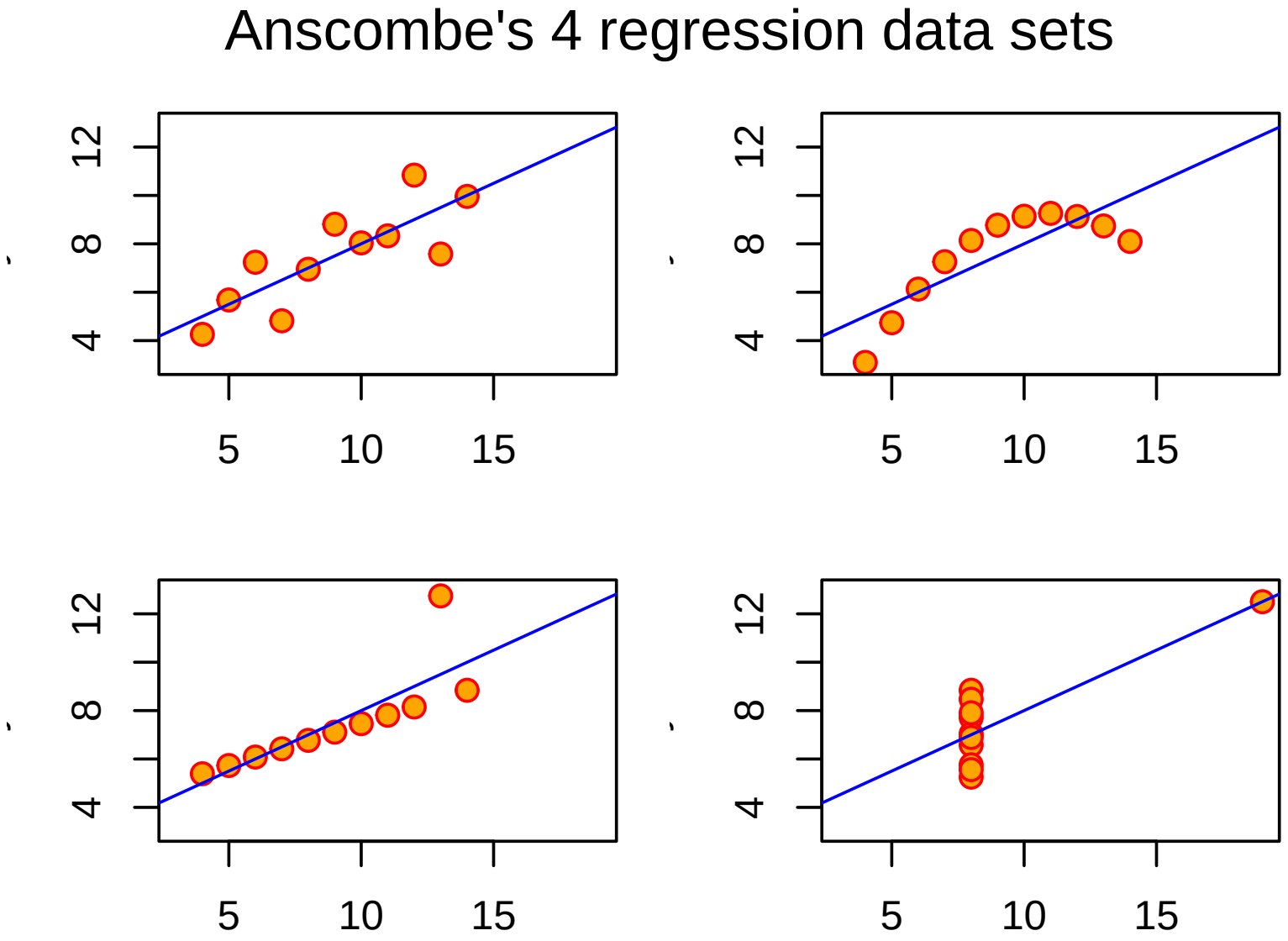
The techniques we will consider are mainly graphical. Graphs are a fundamental tool for statistical practice and in particular for model assessment.

We start by recalling Anscombe's quartet. The code that follows is from the `R` documentation of `anscombe`:

```
## Analysis of Variance Table
##
## Response: y1
##           Df Sum Sq Mean Sq F value  Pr(>F)
## x1         1 27.510 27.5100   17.99 0.00217 **
## Residuals  9 13.763  1.5292
## ---
## Signif. codes:
## 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
## Analysis of Variance Table
##
## Response: y2
##           Df Sum Sq Mean Sq F value   Pr(>F)
## x2         1 27.500 27.5000  17.966 0.002179 **
## Residuals  9 13.776  1.5307
## ---
## Signif. codes:
## 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
## Analysis of Variance Table
##
## Response: y3
##           Df Sum Sq Mean Sq F value   Pr(>F)
## x3         1 27.470 27.4700  17.972 0.002176 **
## Residuals  9 13.756  1.5285
## ---
## Signif. codes:
## 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
## Analysis of Variance Table
##
## Response: y4
##           Df Sum Sq Mean Sq F value   Pr(>F)
## x4         1 27.490 27.4900  18.003 0.002165 **
## Residuals  9 13.742  1.5269
## ---
```

```
##                    lm1      lm2       lm3       lm4
## (Intercept) 3.0000909 3.000909 3.0024545 3.0017273
## x1          0.5000909 0.500000 0.4997273 0.4999091

## $lm1
##               Estimate Std. Error  t value    Pr(>|t|)
## (Intercept) 3.0000909  1.1247468 2.667348 0.025734051
## x1          0.5000909  0.1179055 4.241455 0.002169629
##
## $lm2
##             Estimate Std. Error  t value    Pr(>|t|)
## (Intercept) 3.000909  1.1253024 2.666758 0.025758941
## x2          0.500000  0.1179637 4.238590 0.002178816
##
## $lm3
##               Estimate Std. Error  t value    Pr(>|t|)
## (Intercept) 3.0024545  1.1244812 2.670080 0.025619109
## x3          0.4997273  0.1178777 4.239372 0.002176305
##
## $lm4
##               Estimate Std. Error  t value    Pr(>|t|)
## (Intercept) 3.0017273  1.1239211 2.670763 0.025590425
## x4          0.4999091  0.1178189 4.243028 0.002164602
```


Anscombe's 4 regression data sets
4
8
12
5
10
15

Facts About Residuals

Facts About Residuals

We have assumed that the errors $\epsilon_i, i = 1, \ldots, n$ have a centered Gaussian distribution with constant variance σ^2 and are independent.

The residuals are defined as

$$\hat{\epsilon}_i = y_i - \hat{y}_i,$$

the difference between the observed and the predicted values for $x = x_i$.

Unlike the errors, **the residuals are not independent and do not have constant variance**.

They cannot be independent because we have shown that $\sum_i \hat{\epsilon}_i = 0$ and also that $\sum_i \hat{\epsilon}_i x_i = 0$.

Recall that the regression parameters are given by

$$\hat{\beta} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}$$

and once we have these parameters, the fitted values are given by

$$\hat{\mathbf{Y}} = \mathbf{X}\hat{\beta} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}.$$

The matrix $\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'$ is usually denoted by $\mathbf{H}$ and is known as the *hat* matrix, because it carries the observed vector $\mathbf{y}$ into the fitted values vector $\hat{\mathbf{y}}$.

$$\mathbf{H}\mathbf{y} = \hat{\mathbf{y}}$$

If h_{ij} are the elements of matrix $\mathbf{H}$ then

$$\hat{y}_i = \sum_j h_{ij} y_j.$$

Therefore, we can think of the h_{ij} as the 'weights' needed to go from the observed values to the regression values, and the bigger h_{ij} is, the more influential the observed value y_j will be in the determination of $\hat{y}_i$.

So the hat matrix gives a measure of the 'leverage' of the observations on the fitted model.

In general, the greatest impact of y_i occurs for $\hat{y}_i$ and hence we will focus on the diagonal elements of $\mathbf{H}$.

The **leverage** h_{ii} is the i-th entry in the diagonal of $\mathbf{H}$.

Observe that

$$\begin{aligned} Cov(\hat{\boldsymbol{\epsilon}}) &= Cov(\mathbf{Y} - \hat{\mathbf{Y}}) = Cov(\mathbf{Y} - \mathbf{HY}) \\ &= Cov((\mathbf{I} - \mathbf{H})\mathbf{Y}) = (\mathbf{I} - \mathbf{H})\sigma^2\mathbf{I}(\mathbf{I} - \mathbf{H})' \\ &= \sigma^2(\mathbf{I} - \mathbf{H})(\mathbf{I} - \mathbf{H})'. \end{aligned}$$

Now, since $\mathbf{H}$ is symmetric, $\mathbf{I} - \mathbf{H}$ is also symmetric and it is easy to see that $(\mathbf{I} - \mathbf{H})^2 = \mathbf{I} - \mathbf{H}$ so $\mathbf{I} - \mathbf{H}$ is also idempotent.

Therefore, we get that $Var(\hat{\epsilon}_i) = \sigma^2(\hat{\epsilon}_i) = \sigma^2(1 - h_{ii})$.

Since the h_{ii} need not be equal, we see that the residuals do not have the same variance.

Also, since $\mathbf{H}$ need not be a diagonal matrix, the $\hat{\epsilon}_i$ are usually correlated and not independent.

It is possible to prove that $0 \leq h_{ii} \leq 1$ and that

$$h_{ii} = \frac{1}{n} + \frac{(x_i - \bar{x})^2}{\sum_i (x_i - \bar{x})^2}.$$

The **standardized** residuals are defined as

$$t_i = \frac{\hat{\epsilon}_i}{\hat{\sigma}(1 - h_{ii})^{1/2}}$$

where $\hat{\sigma}$ is the estimated error standard deviation.

Homoscedasticity and Linearity

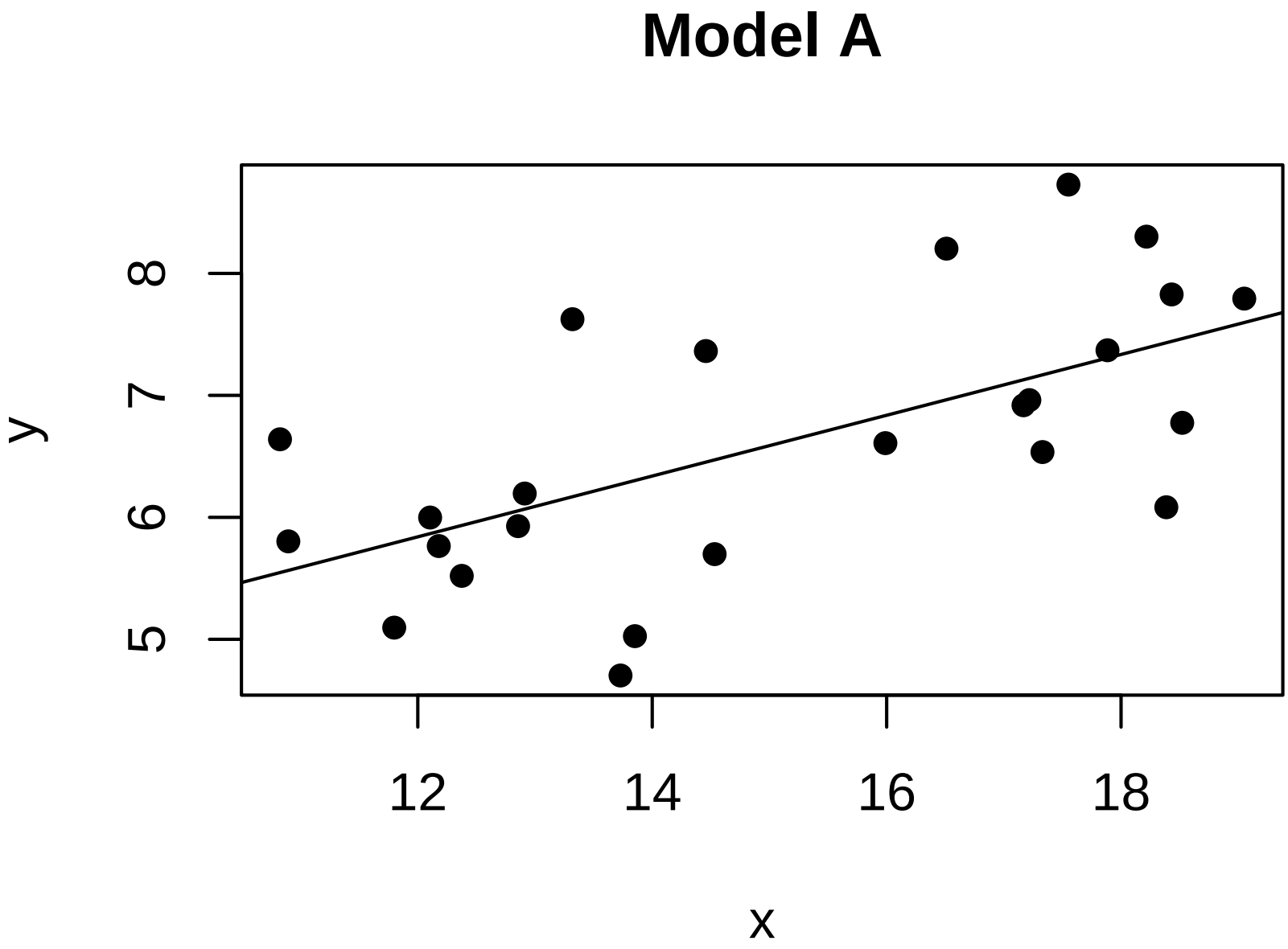
Homoscedasticity and Linearity

The first graph that is usually drawn for model evaluation is a plot of residuals against fitted values

If the model assumptions are correct and we have captured as much variability as possible with the model, in this graph we would expect to see no patterns, but points scattered at random over the plotting region.

The presence of patterns may indicate that the assumption of equal variance (homoscedasticity) does not hold, or that there are still possible improvements in the model.

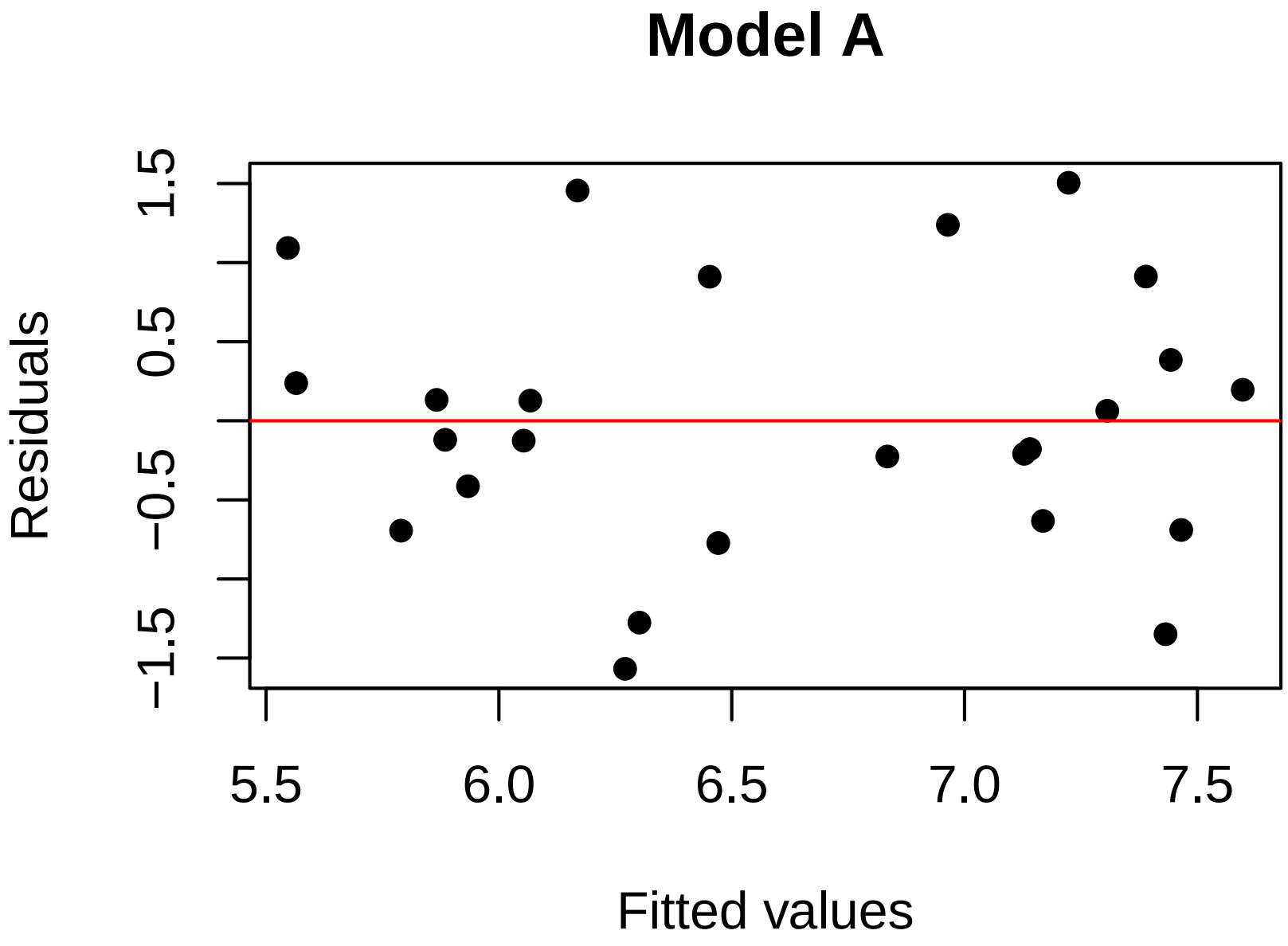
Let us see an example of this situation with simulated data. This will be `modelA`.

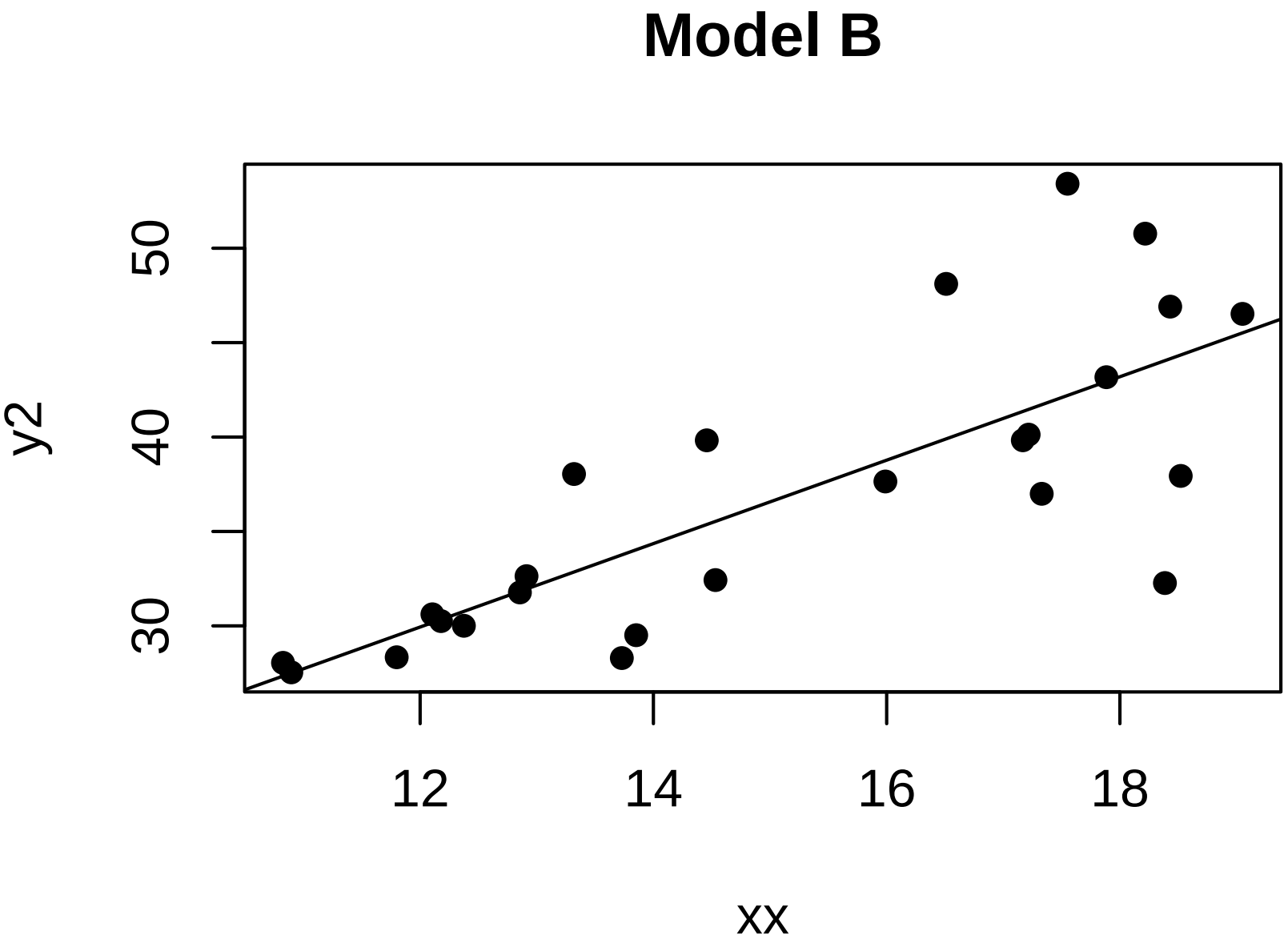

Model A
y
5
6
7
8
12
14
16
18
x

Homoscedasticity and Linearity

```
summary(modelA)
```

```
##
## Call:
## lm(formula = y1 ~ xx)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -1.5680 -0.6330 -0.1202  0.3848  1.5047
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)  2.84963    0.99632   2.860 0.008853 **
## xx           0.24921    0.06488   3.841 0.000834 ***
## ---
## Signif. codes:
## 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.8659 on 23 degrees of freedom
## Multiple R-squared:  0.3908, Adjusted R-squared:  0.3643
## F-statistic: 14.76 on 1 and 23 DF,  p-value: 0.0008336
```

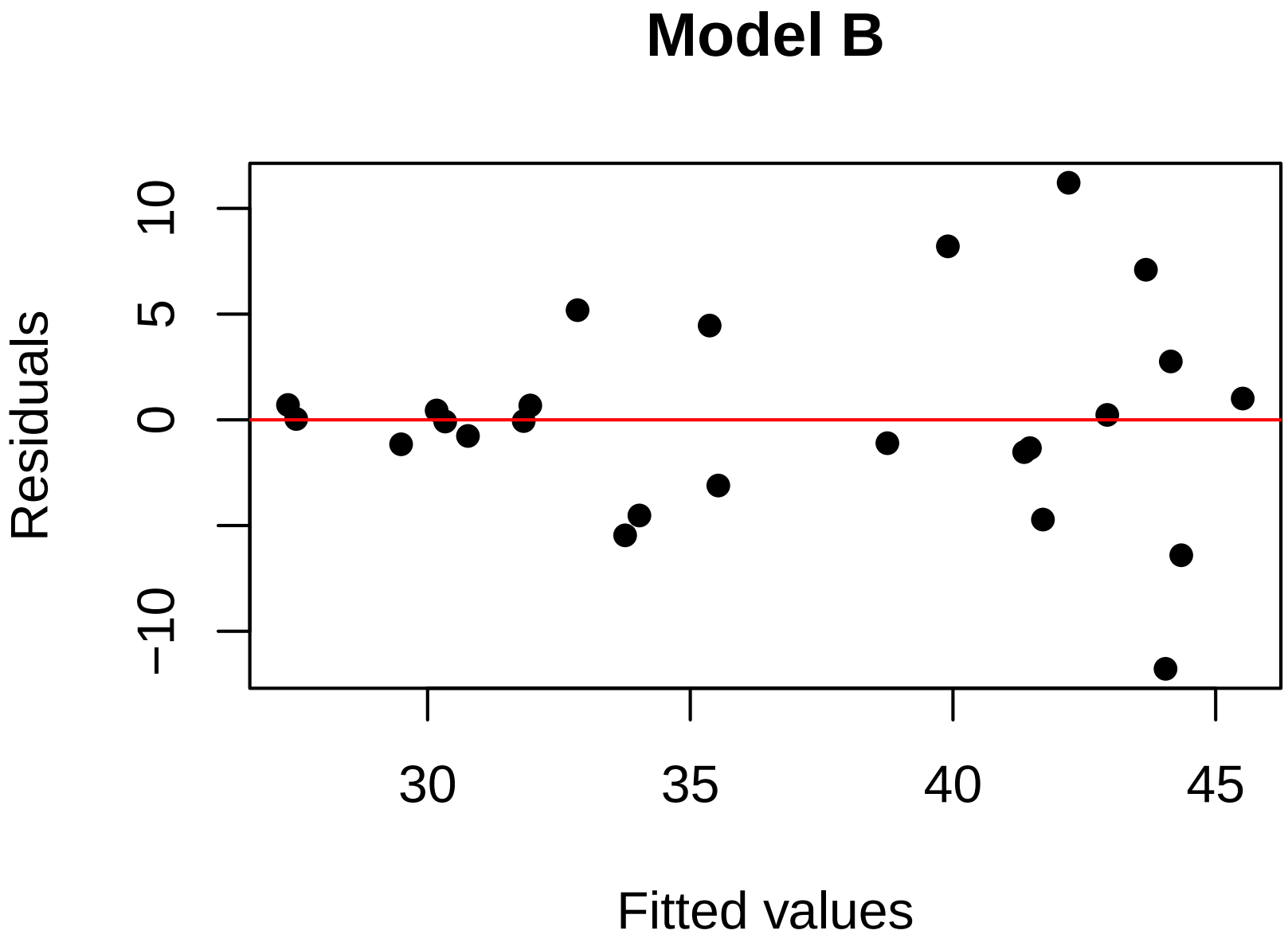

Model A
Residuals
1.5
0.5
−0.5
−1.5
5.5
6.0
6.5
7.0
7.5
Fitted values

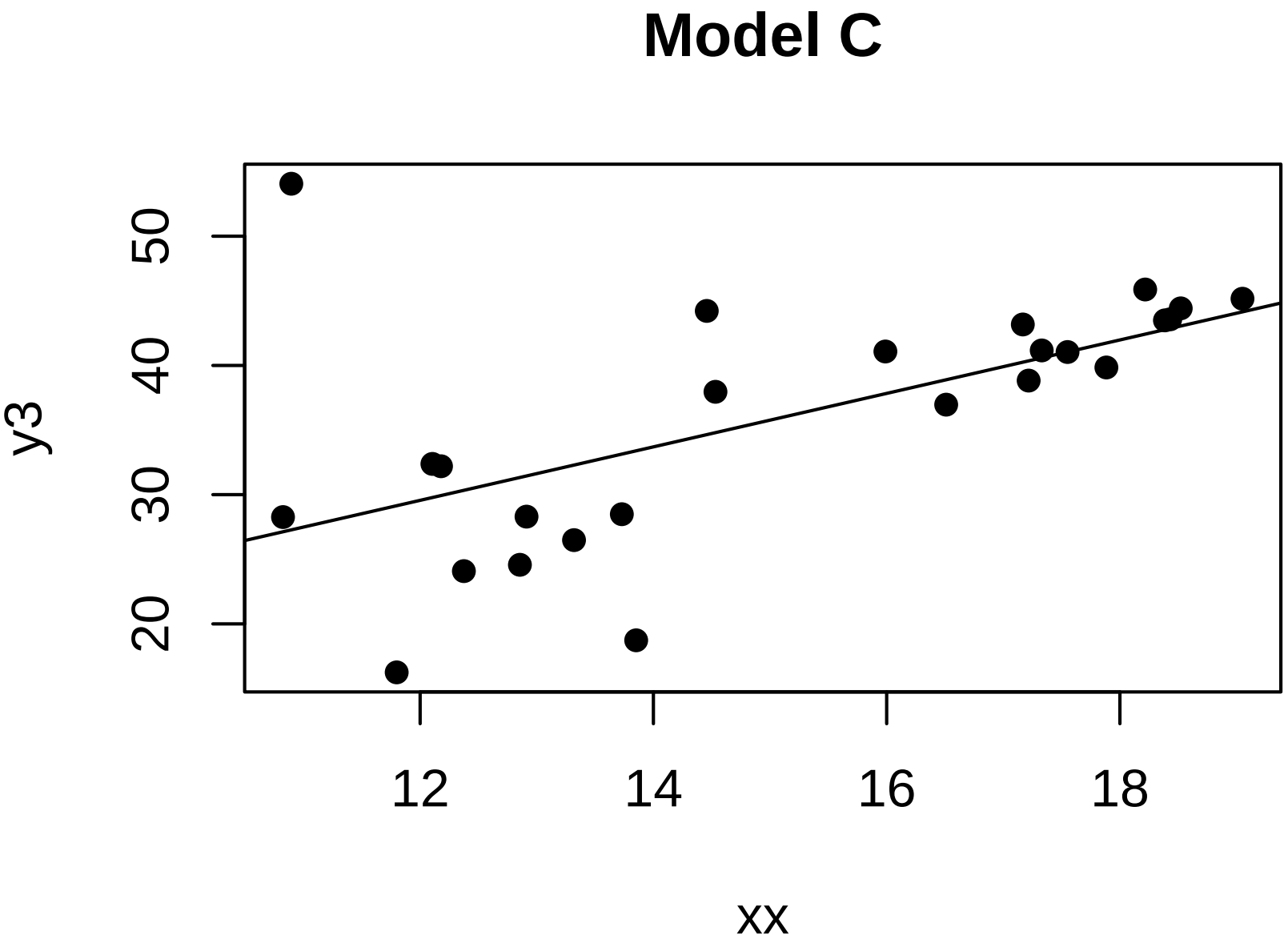

Model B
y2
30
40
50
12
14
16
18
xx

Homoscedasticity and Linearity

```
summary(modelB)
```

```
##
## Call:
## lm(formula = y2 ~ xx)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -11.7769  -1.5265  -0.0589   1.0082  11.2117
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)   3.4322     5.7244   0.600    0.555
## xx            2.2090     0.3727   5.926 4.84e-06 ***
## ---
## Signif. codes:
## 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 4.975 on 23 degrees of freedom
## Multiple R-squared:  0.6043, Adjusted R-squared:  0.5871
## F-statistic: 35.12 on 1 and 23 DF,  p-value: 4.843e-06
```

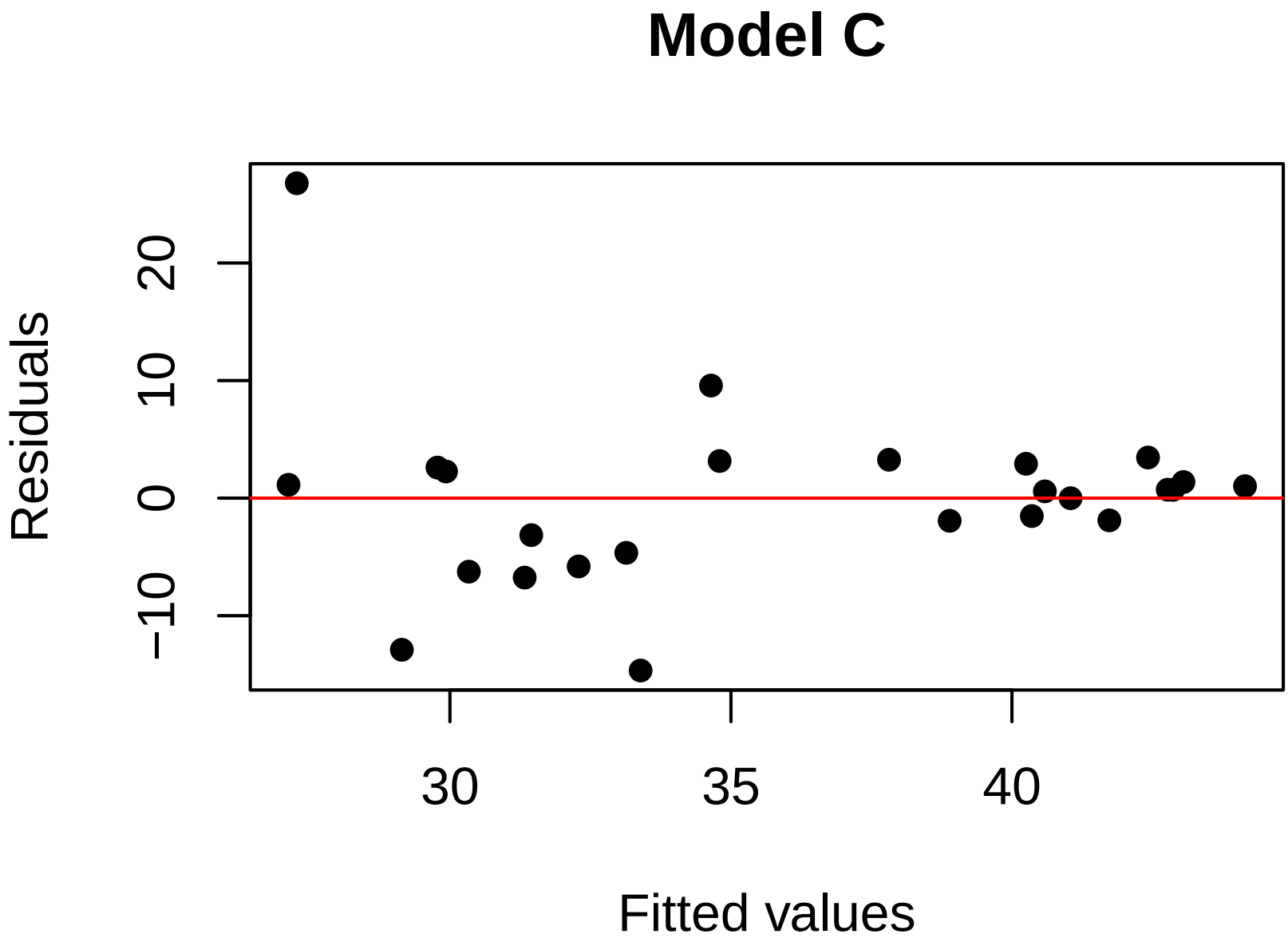

Model B
Residuals
10
5
0
−10
30
35
40
45
Fitted values


Model C
y3
20
30
40
50
12
14
16
18
xx

Homoscedasticity and Linearity

```
summary(modelC)
```

```
##
## Call:
## lm(formula = y3 ~ xx)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -14.6647  -3.1477   0.7031   2.6000  26.7857
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)   4.7352     9.0057   0.526   0.6041
## xx            2.0687     0.5864   3.528   0.0018 **
## ---
## Signif. codes:
## 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 7.826 on 23 degrees of freedom
## Multiple R-squared:  0.3511, Adjusted R-squared:  0.3229
## F-statistic: 12.45 on 1 and 23 DF,  p-value: 0.001802
```


Model C
Residuals
20
10
0
−10
30
35
40
Fitted values

In both cases we have a 'funnel' shape, although with different orientations. This is an indication that the variance is not constant.

A possible way to deal with this problem is to transform the data. Useful transformations in this case are the Box-Cox transformations. We won't go into any detail about this but for positive data the transformations are given by

$$T_\lambda(y) = \begin{cases} \frac{y^\lambda - 1}{\lambda} & \text{if } \lambda \neq 0 \\ \log(y) & \text{if } \lambda = 0 \end{cases}$$

The command `boxcox` in `R` calculates the optimal transformation for a given data set.

The graphs of residuals against fitted values are also useful to detect cases in which the model does not explain all the structure present in the data.

Example Q

As an example let us consider a quadratic relation between two variables that we try to model as a linear relation.

```
set.seed(4567)
xx <- runif(25,10,20)
zz <- rnorm(25,sd=4)
y4 <-  2 + 1.3*xx+ 3*(xx-10)^2+zz
modelD <- lm(y4~xx)
```

Homoscedasticity and Linearity

```
summary(modelD)
```

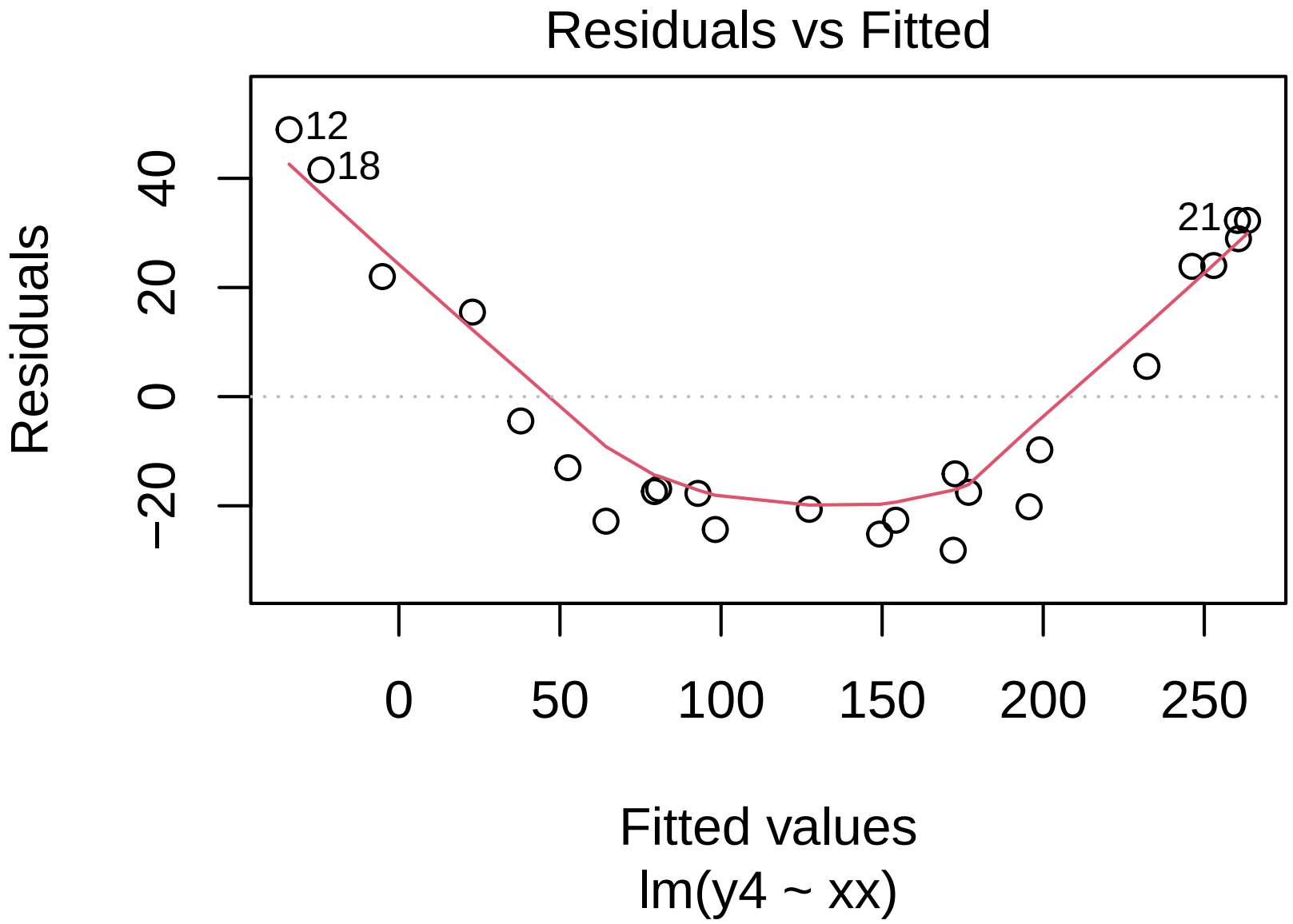
```
##
## Call:
## lm(formula = y4 ~ xx)
##
## Residuals:
##    Min     1Q Median     3Q    Max
## -28.14 -20.18 -13.02  23.87  48.93
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept) -350.746     26.814  -13.08 3.88e-12 ***
## xx            31.569      1.718   18.37 3.06e-15 ***
## ---
## Signif. codes:
## 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 25.13 on 23 degrees of freedom
## Multiple R-squared:  0.9362, Adjusted R-squared:  0.9334
## F-statistic: 337.5 on 1 and 23 DF,  p-value: 3.057e-15
```

In the summary for the regression we see that slope and intersect are significant with a very low p-value and that the coefficient of determination R^2 has a (high) value of 0.936.

However, if we look at the summary data for the residuals, we see that the values do not correspond to a symmetric distribution, as one would expect if they followed a (centered) normal distribution.

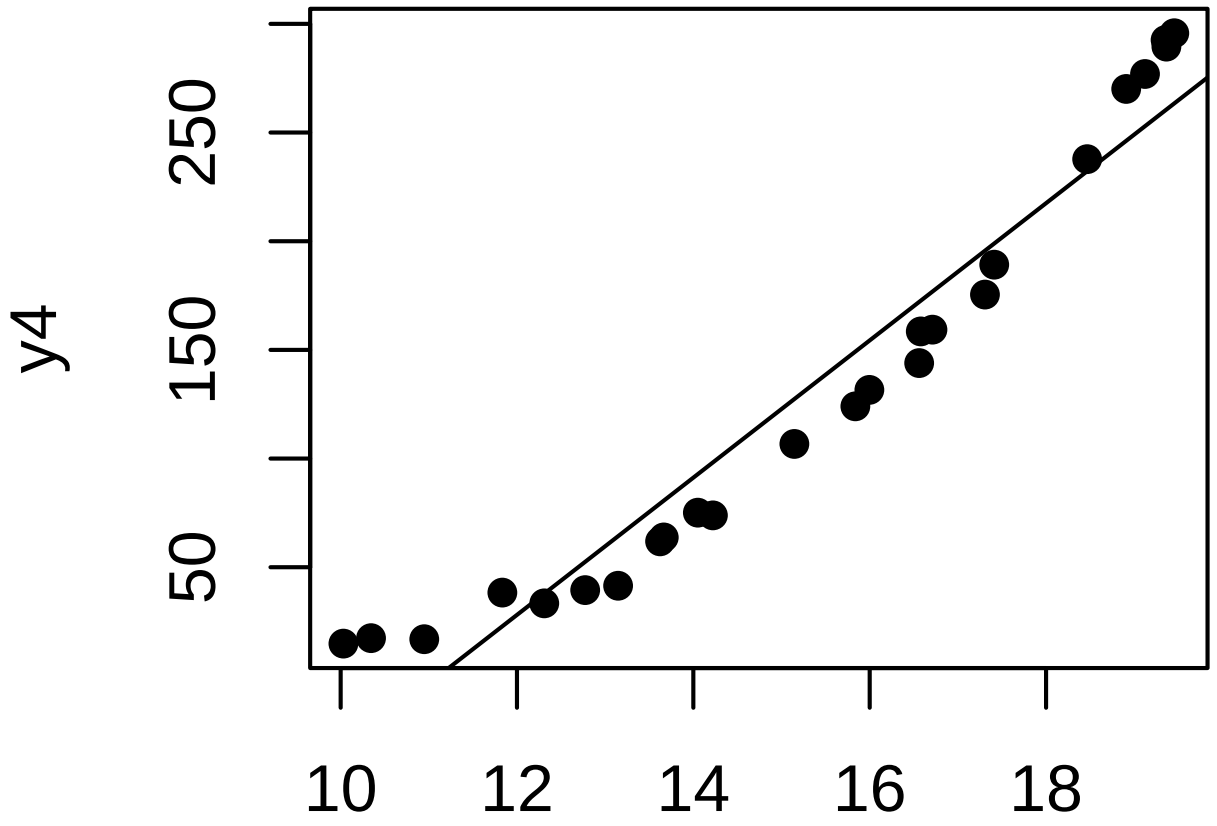
Homoscedasticity and Linearity

```
plot(modelD, which = 1)
```



Indeed, if we had looked at the data in the first place -something one should always do- we would have seen that a linear relation is not adequate for this data.

```
plot(xx,y4,pch=16); abline(modelD)
```



We can add a quadratic term to the regression to include this structure into account. We will look at multiple regression in detail later on, but for completeness, let's fit a quadratic model.

```
modelE <- lm(y4~xx+I(xx^2))
summary(modelE)
```

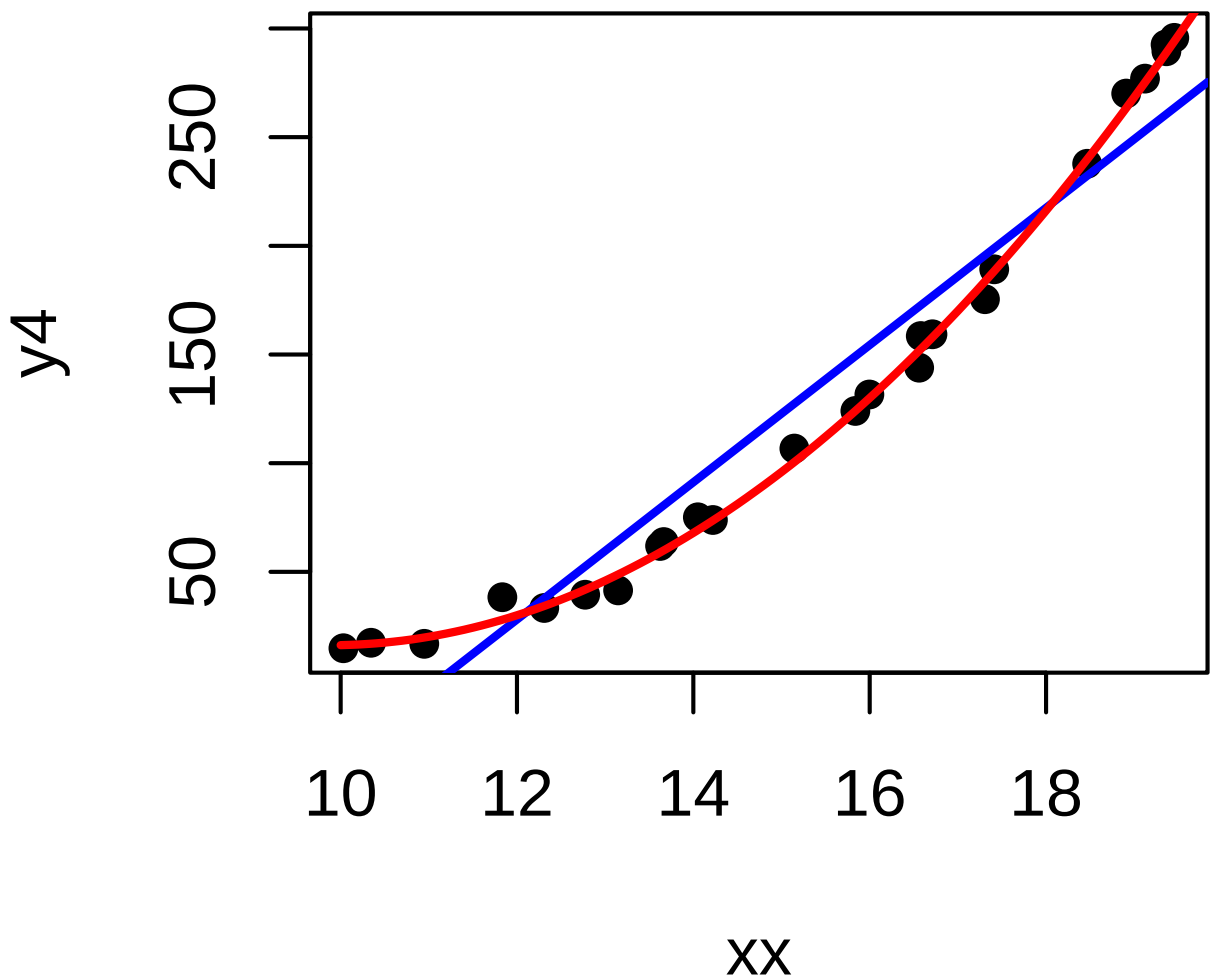
```
##
## Call:
## lm(formula = y4 ~ xx + I(xx^2))
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -9.2420 -1.8221  0.0683  2.8383  9.8580
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept) 309.9679    26.9643   11.50 9.03e-11 ***
## xx          -59.5669     3.6675  -16.24 9.81e-14 ***
## I(xx^2)       3.0235     0.1212   24.95  < 2e-16 ***
## ---
## Signif. codes:
## 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 4.747 on 22 degrees of freedom
## Multiple R-squared:  0.9978, Adjusted R-squared:  0.9976
## F-statistic:  5039 on 2 and 22 DF,  p-value: < 2.2e-16
```

From the summary data for the regression we see that linear and quadratic terms are significant and that the summary data for the residuals is consistent with a symmetric distribution.

Also, the R^2 has increased to 0.998.

Next we plot the data, the regresion line (from the first regression model) and the quadratic curve we have just fitted.

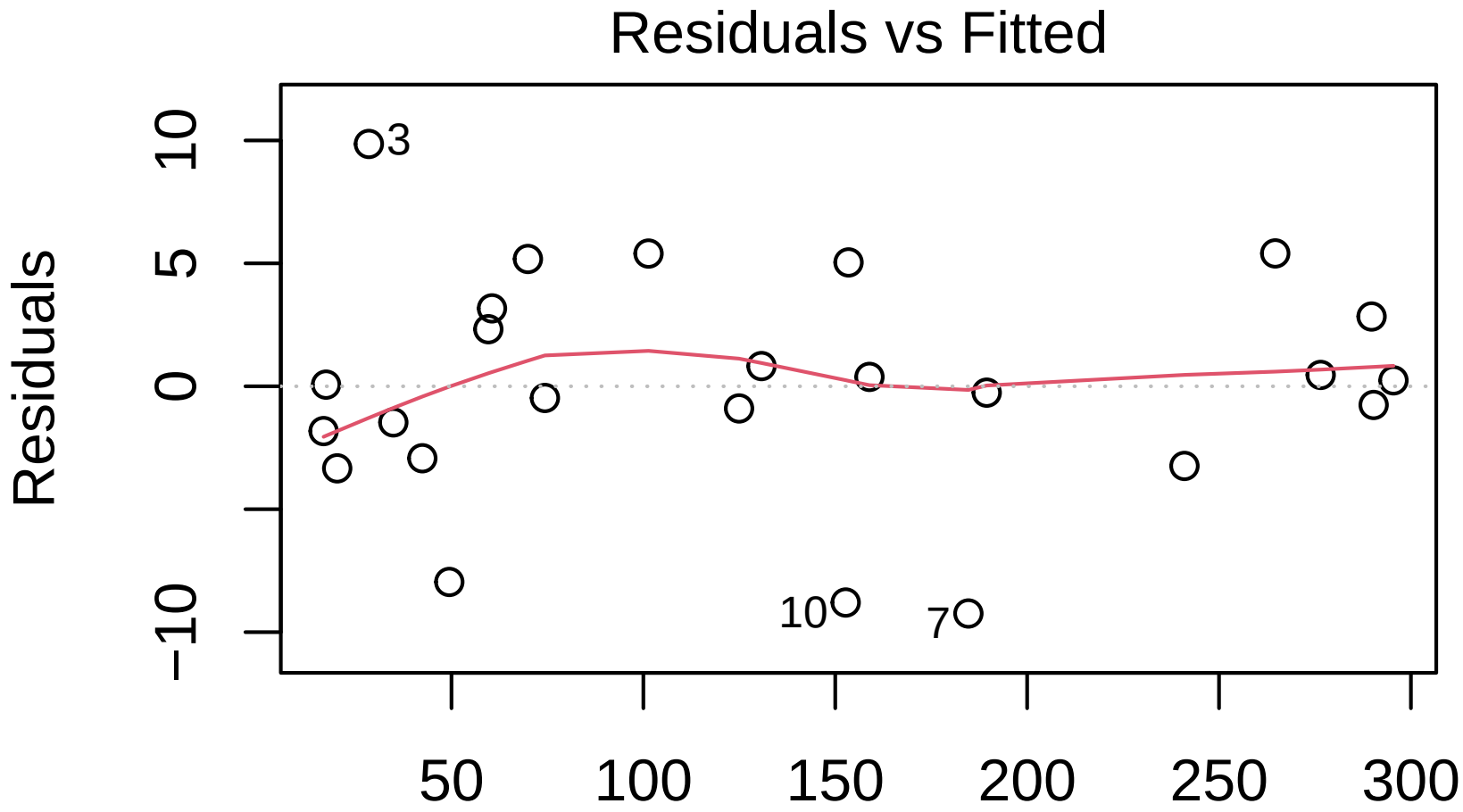
```
plot(xx,y4,pch=16)
abline(modelD, col='blue', lwd=2)
curve(309.99-59.57*x+3.02*x^2,10,20, add=T,
      col='red', lwd=2)
```



Homoscedasticity and Linearity

Finally, the graphs to evaluate the new model look much better than the those for the previous model.

```
plot(modelE, which = 1)
```

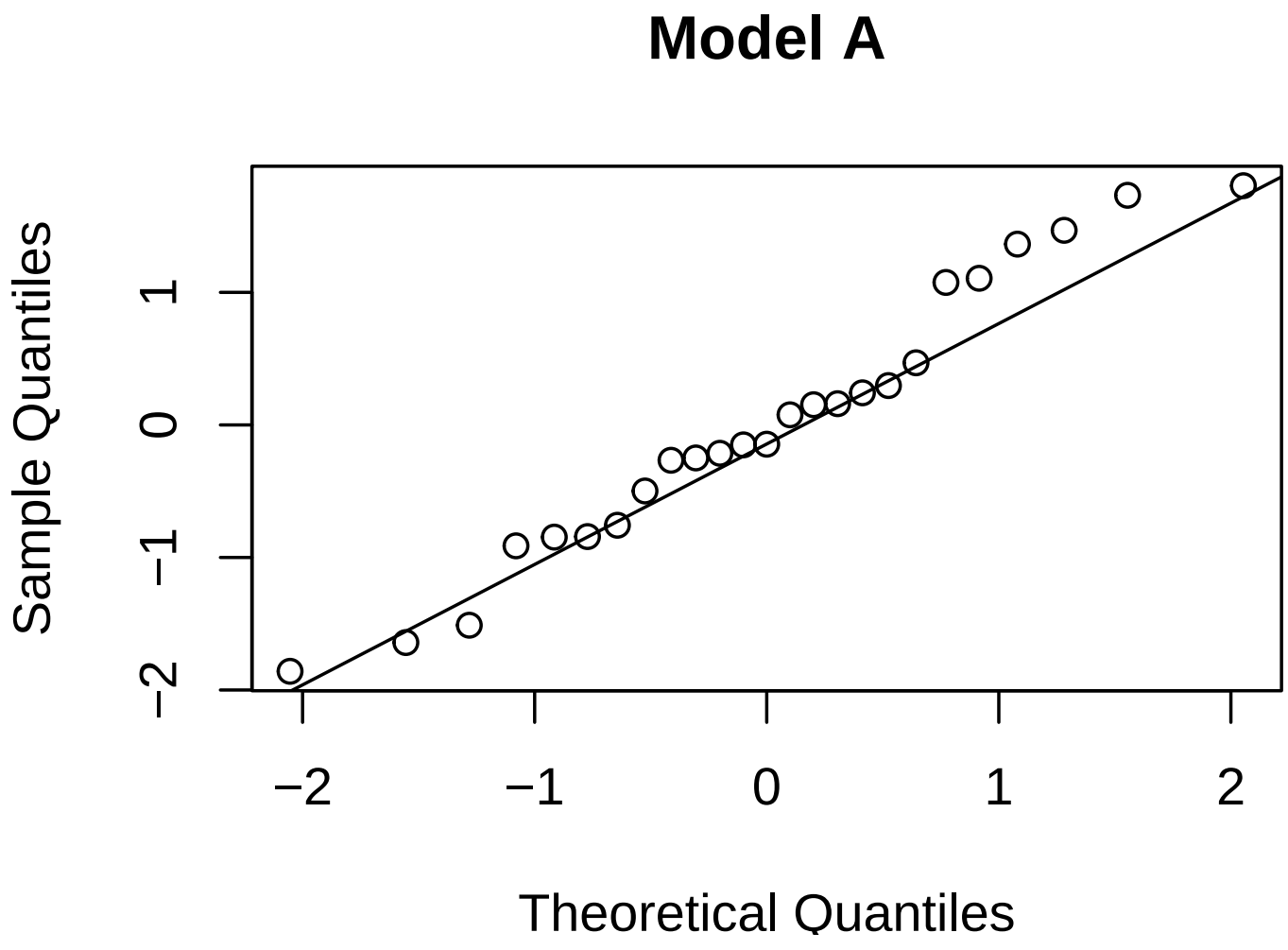


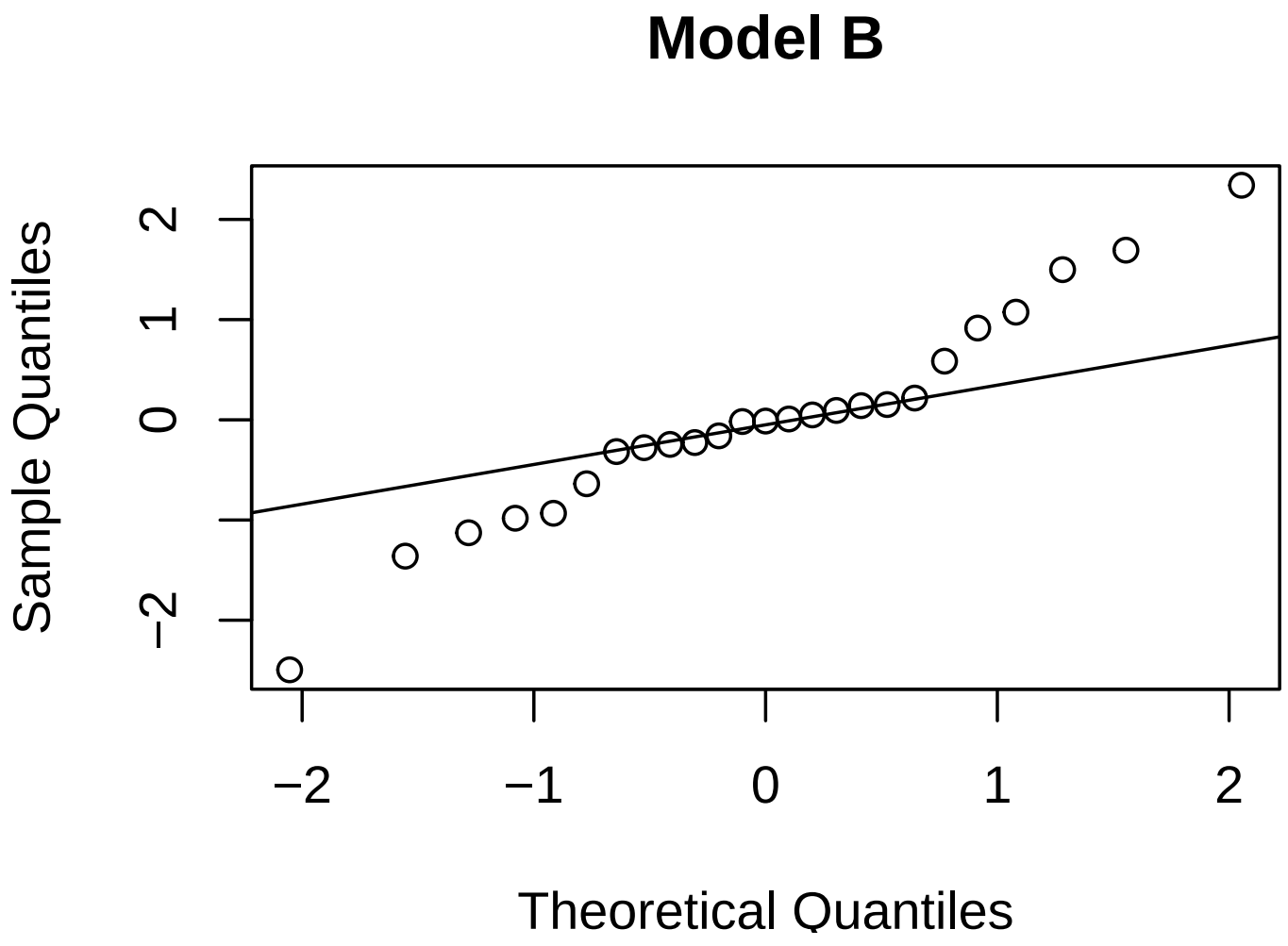
Gaussianity

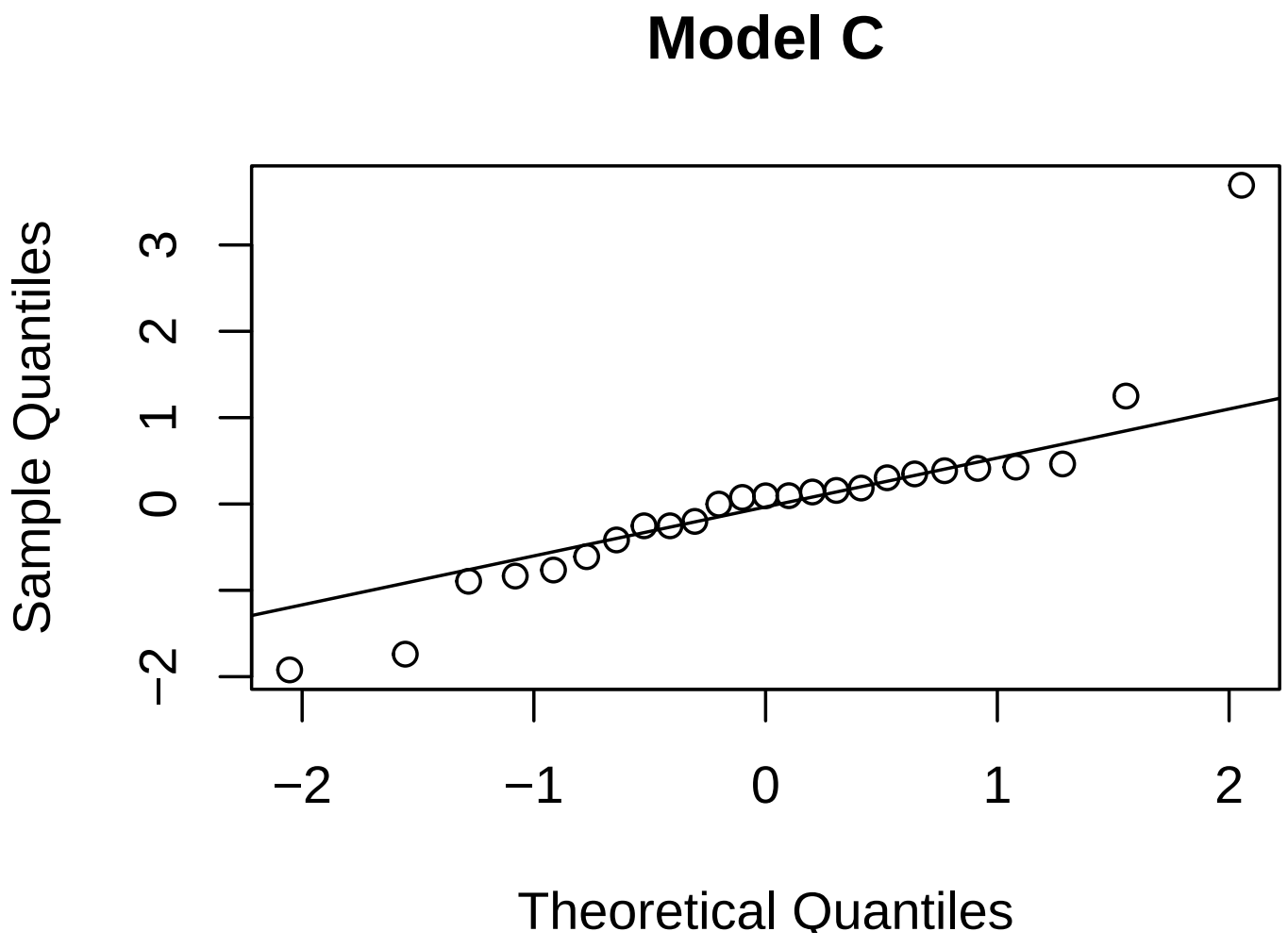
Another important assumption we have made is that the errors have a normal distribution.

To check this assumption it is usual to draw a quantile plot for the residuals. However, since we have seen that the residuals do not have constant variance, it is usual to plot the standardized residuals.

In `R`, standardized residuals are obtained with the `rstandard` command acting on an `lm` object

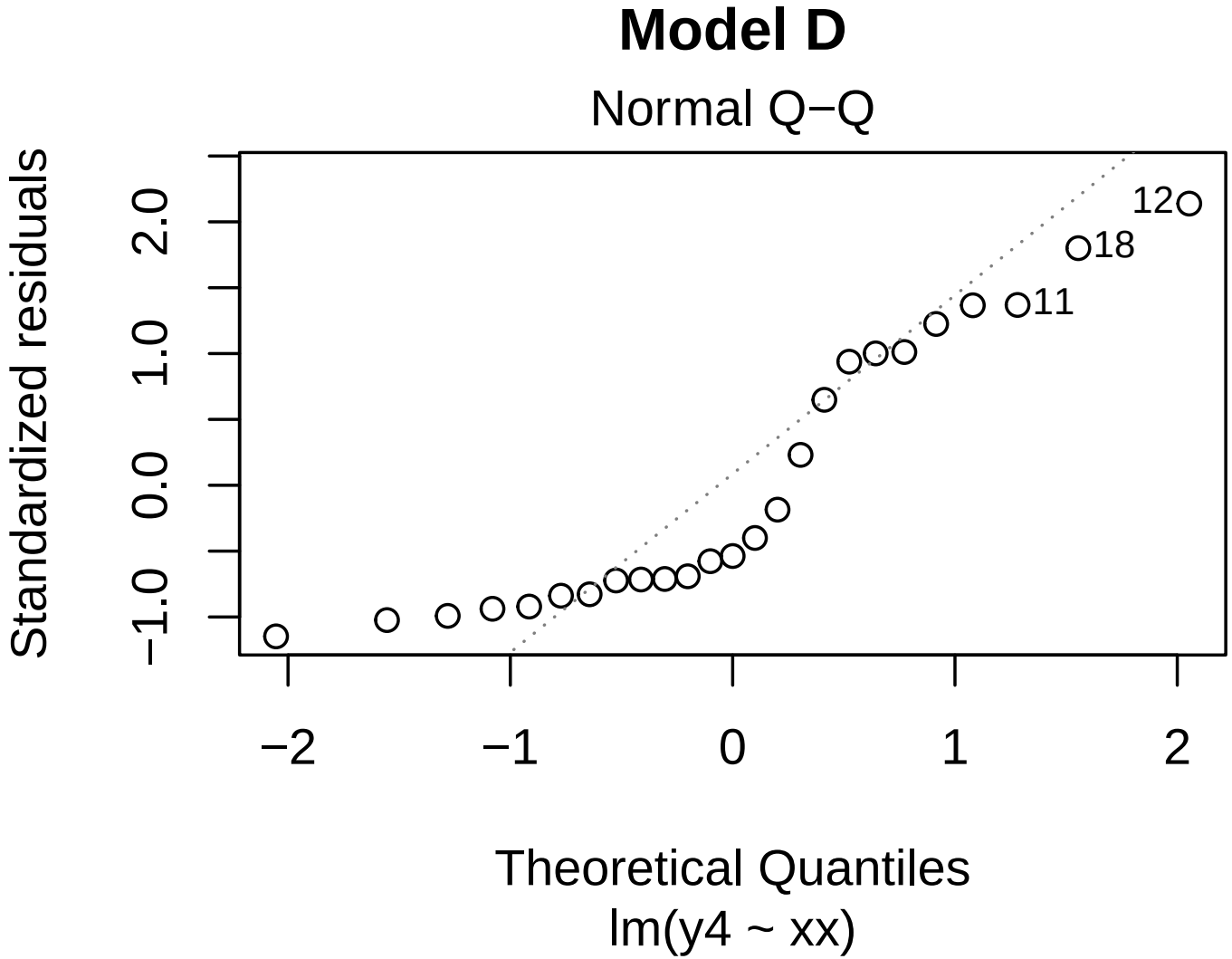

Model A
Sample Quantiles
−2
−1
0
1
−2
−1
0
1
2
Theoretical Quantiles


Model B
Sample Quantiles
−2
0
1
2
−2
−1
0
1
2
Theoretical Quantiles

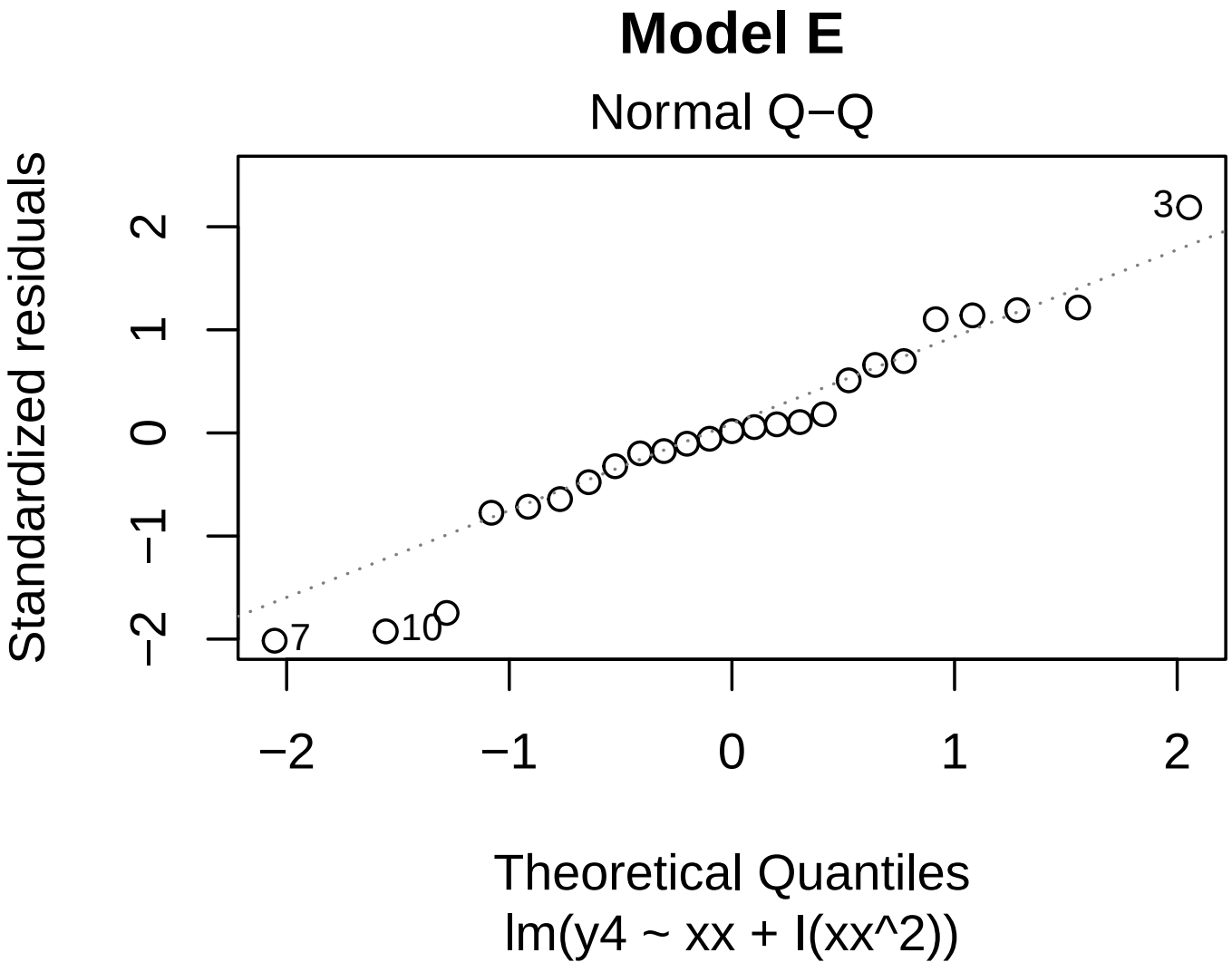

Model C
Sample Quantiles
−2
0
1
2
3
−2
−1
0
1
2
Theoretical Quantiles

Gaussianity: Example Q

Let's go back to example Q and graph the quantiles plots before and after adding the quadratic term.



Gaussianity: Example Q

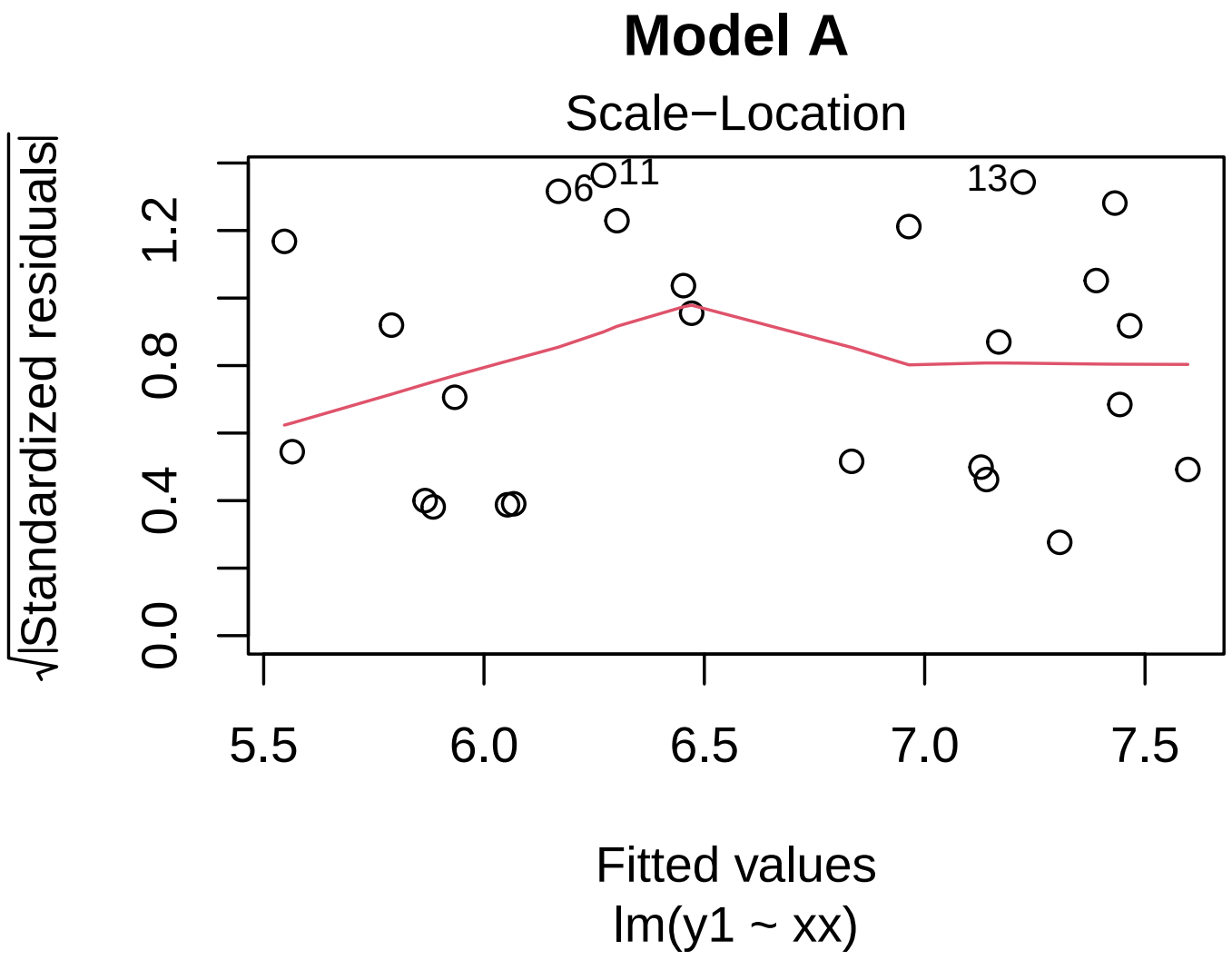


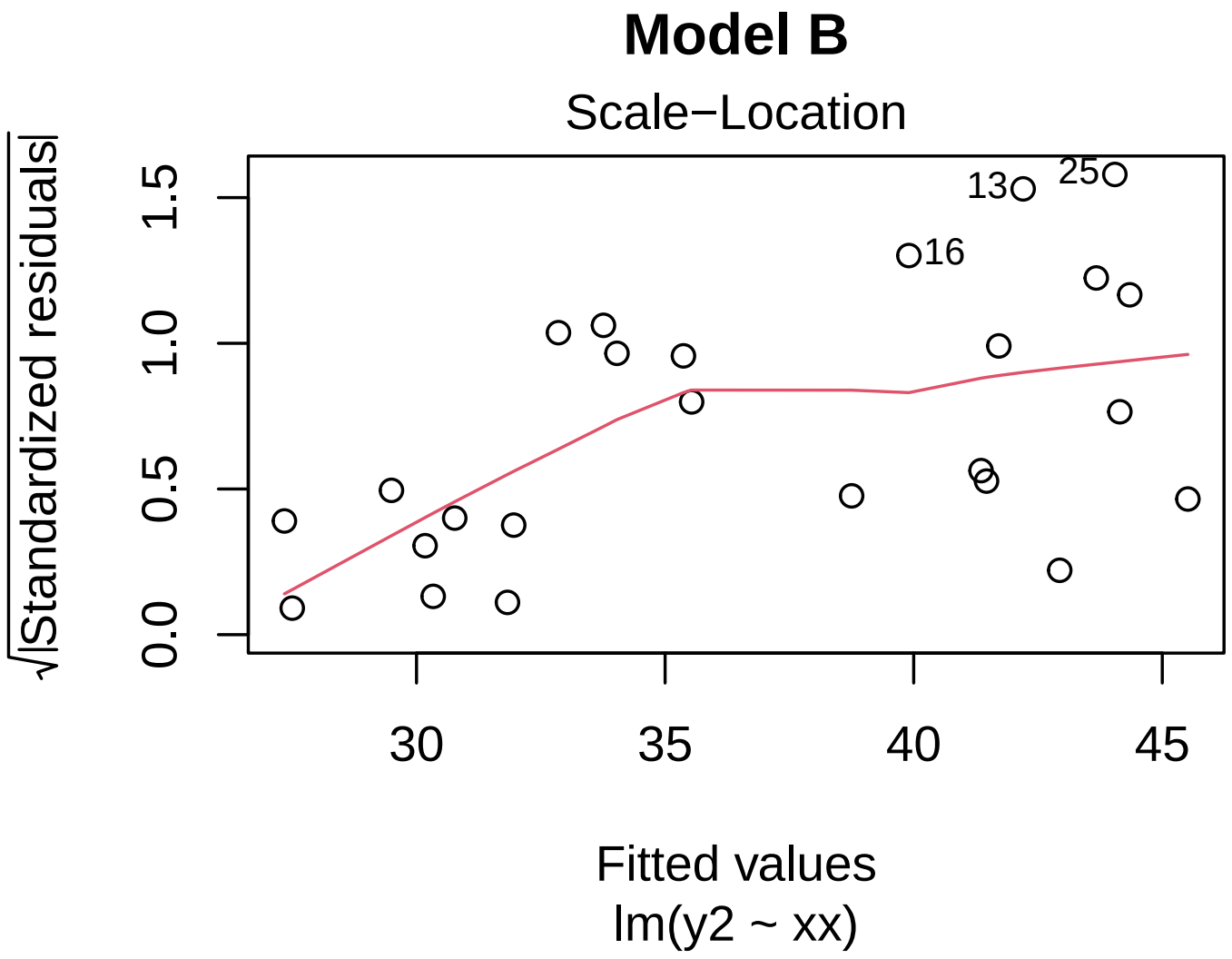
A third graph that is also useful for detecting departures from the assumptions, is similar to the first one on a different scale.

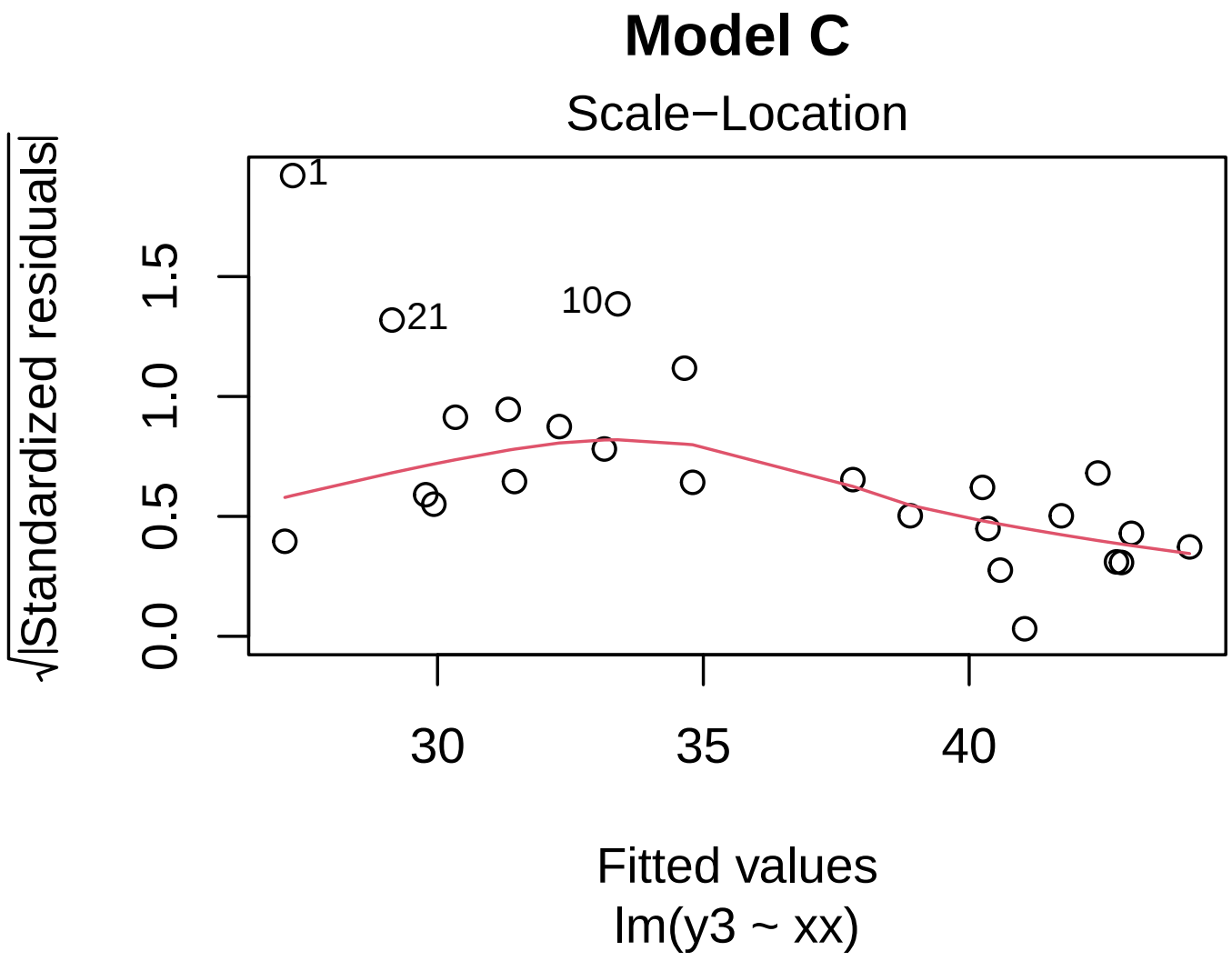
Instead of the residuals, the square root of the absolute value of the standardized residuals is plotted against fitted values, so all values in the y axis are positive.

Again, we expect to see no structure or patterns, but random points scattered on the graph.

Additionally, since the residuals have been standardized, large values indicate possible atypical points.


Model A
Scale−Location
√|Standardized residuals|
0.0
0.4
0.8
1.2
6
11
13
5.5
6.0
6.5
7.0
7.5
Fitted values
lm(y1 ~ xx)

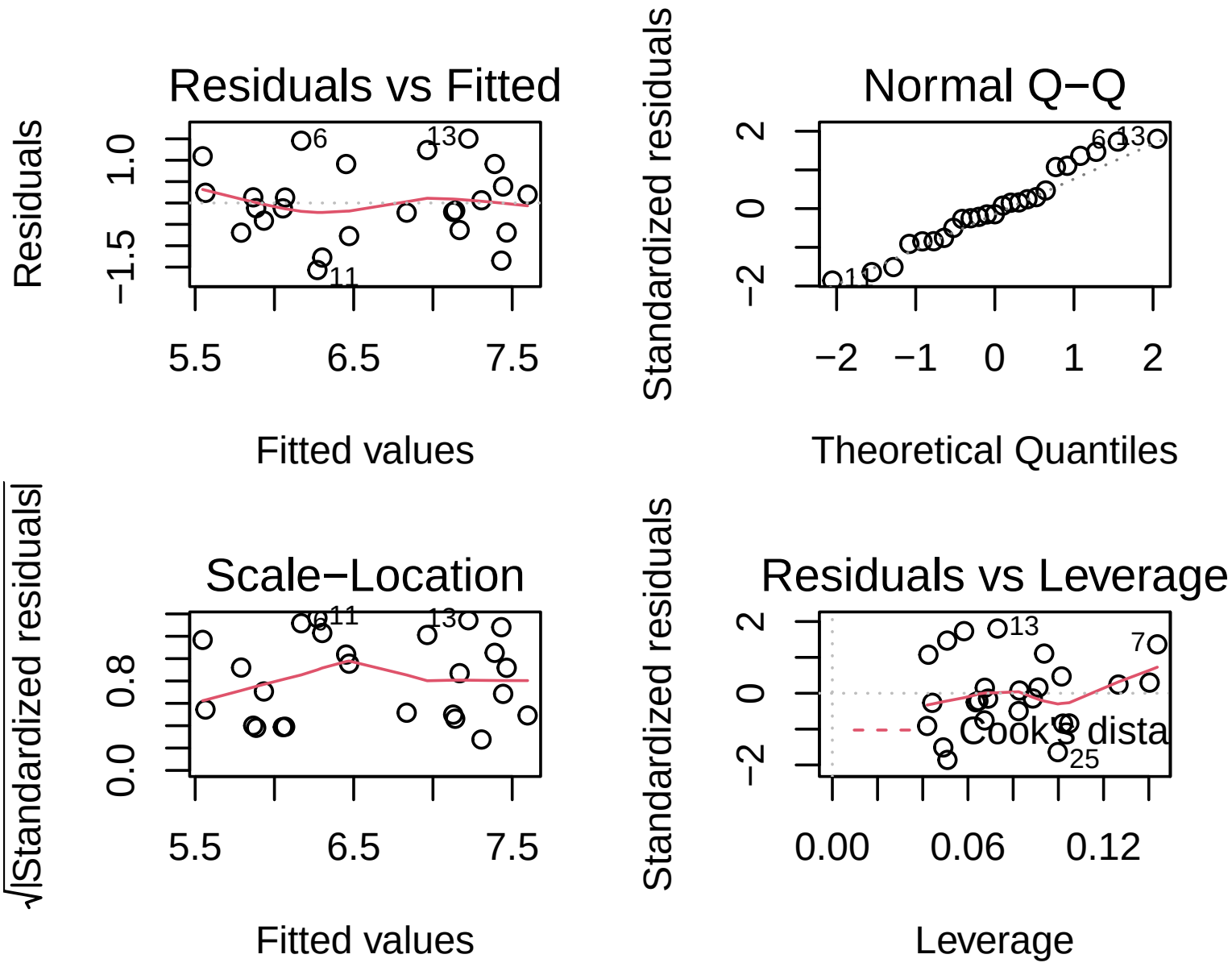

Model B
Scale−Location
√|Standardized residuals|
0.0
0.5
1.0
1.5
13
25
16
30
35
40
45
Fitted values
lm(y2 ~ xx)


Model C
Scale−Location
√|Standardized residuals|
0.0
0.5
1.0
1.5
1
21
10
30
35
40
Fitted values
lm(y3 ~ xx)

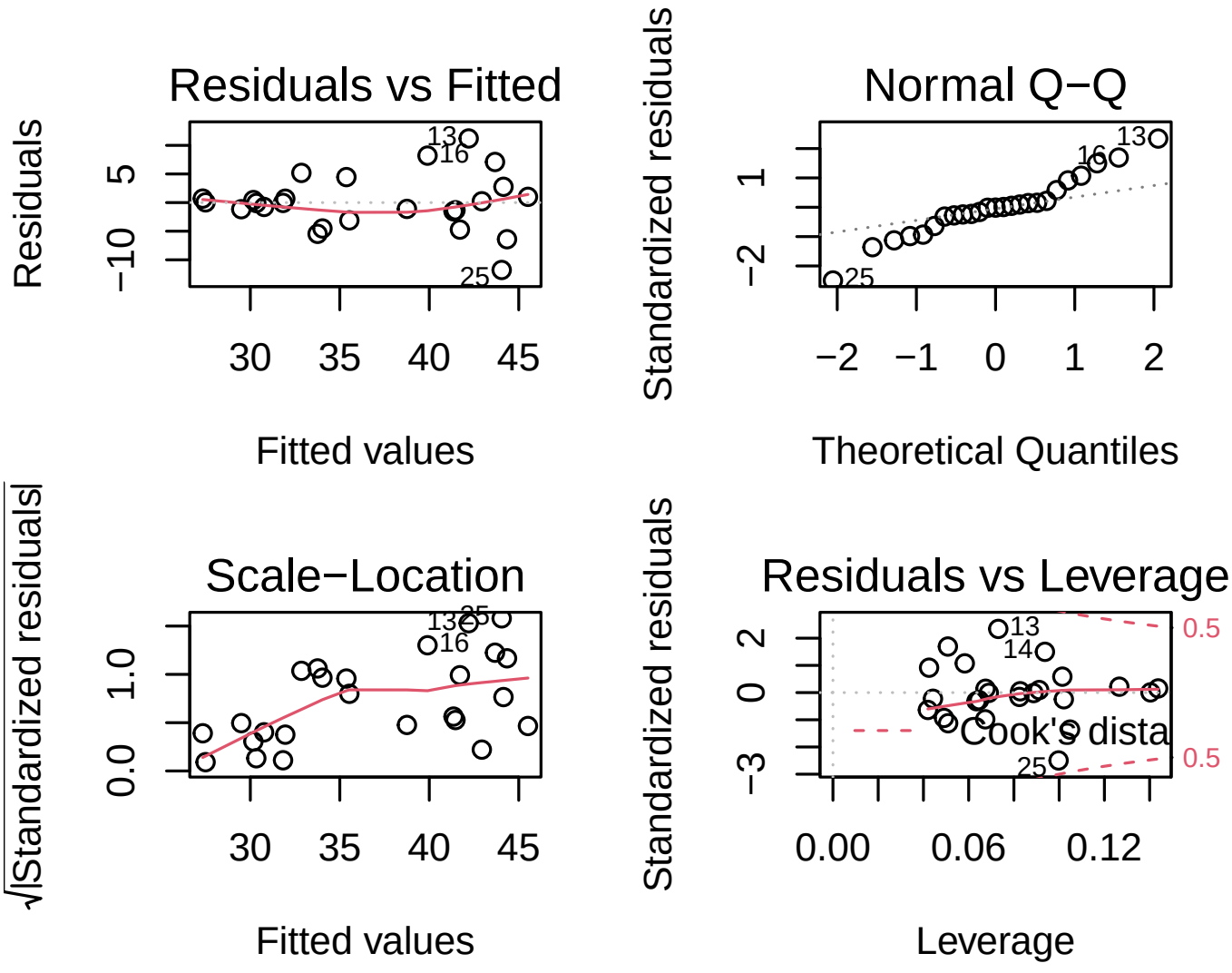
Finally, a graph of standardized residuals against leverage is usually drawn. This plot highlights the values that have highest influence on the parameter estimates.

As we have seen before, these four graphs can be obtained from an `lm` object using the `plot` function if the screen has been previously partitioned into four, as the following instructions illustrate for the first two models we fitted previously.

Diagnostic Plots



Diagnostic Plots



V32: Simple Linear Regression 6: Influential Points and Transformations

Influential and Atypical Points

Atypical points are data that have large residuals in relation to the residuals of the rest of the observations.

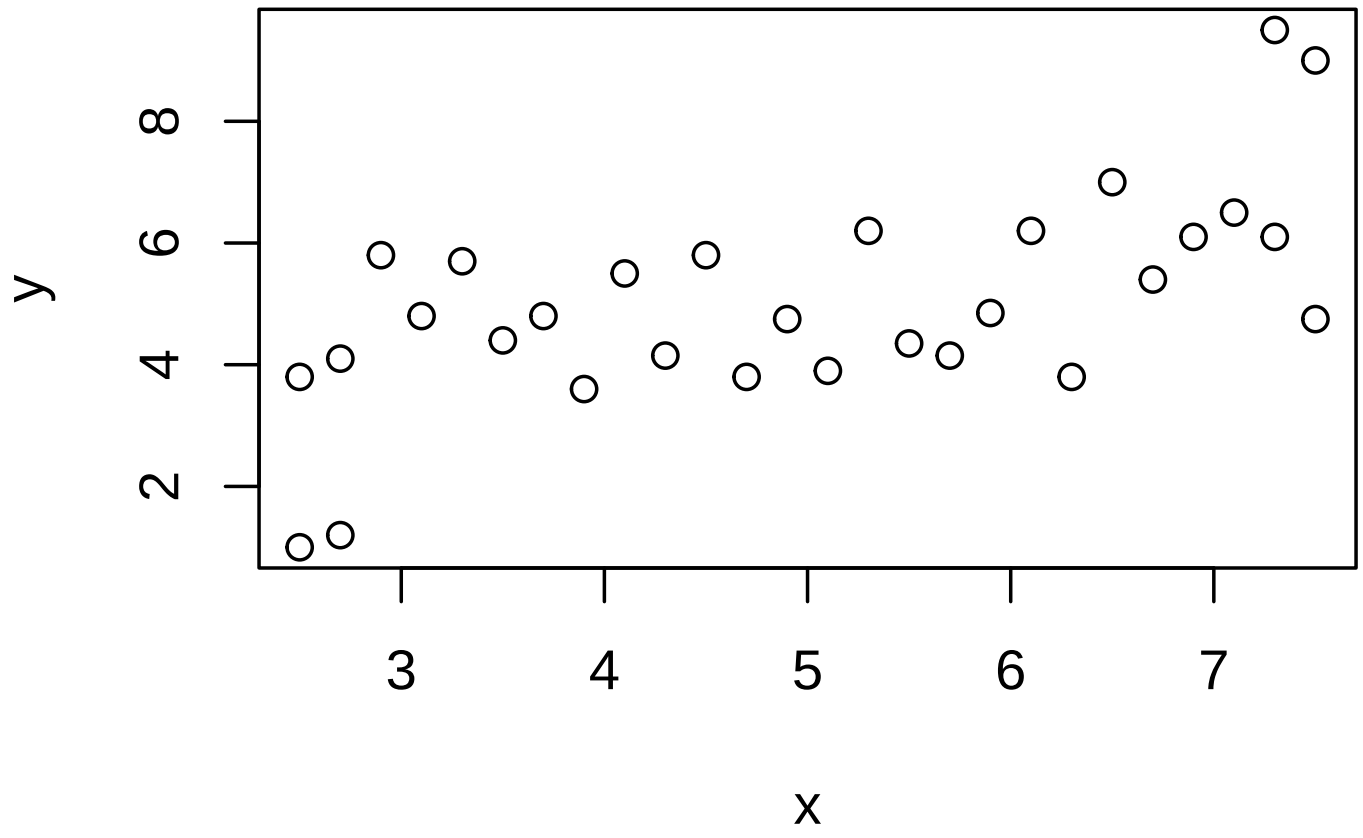
Influential points are points that have a strong influence on the model. By this, we mean that if the model is fitted excluding these points, the model changes substantially.

Let's see an example of the effect of influential points on regression, taken from Chatterjee, Hadi, & Price's book[1].

The following data comes from a study to measure the effect that the rating of the previous program has on the audience of a newscast.

[1] Chatterjee, Hadi & Price *Regression Analysis by Example, 3rd Edition*, Wiley, 1999

```
tv <- read.csv('TV.csv')
plot(tv)
```



The graph shows a possible linear relationship between the variables with a positive slope.

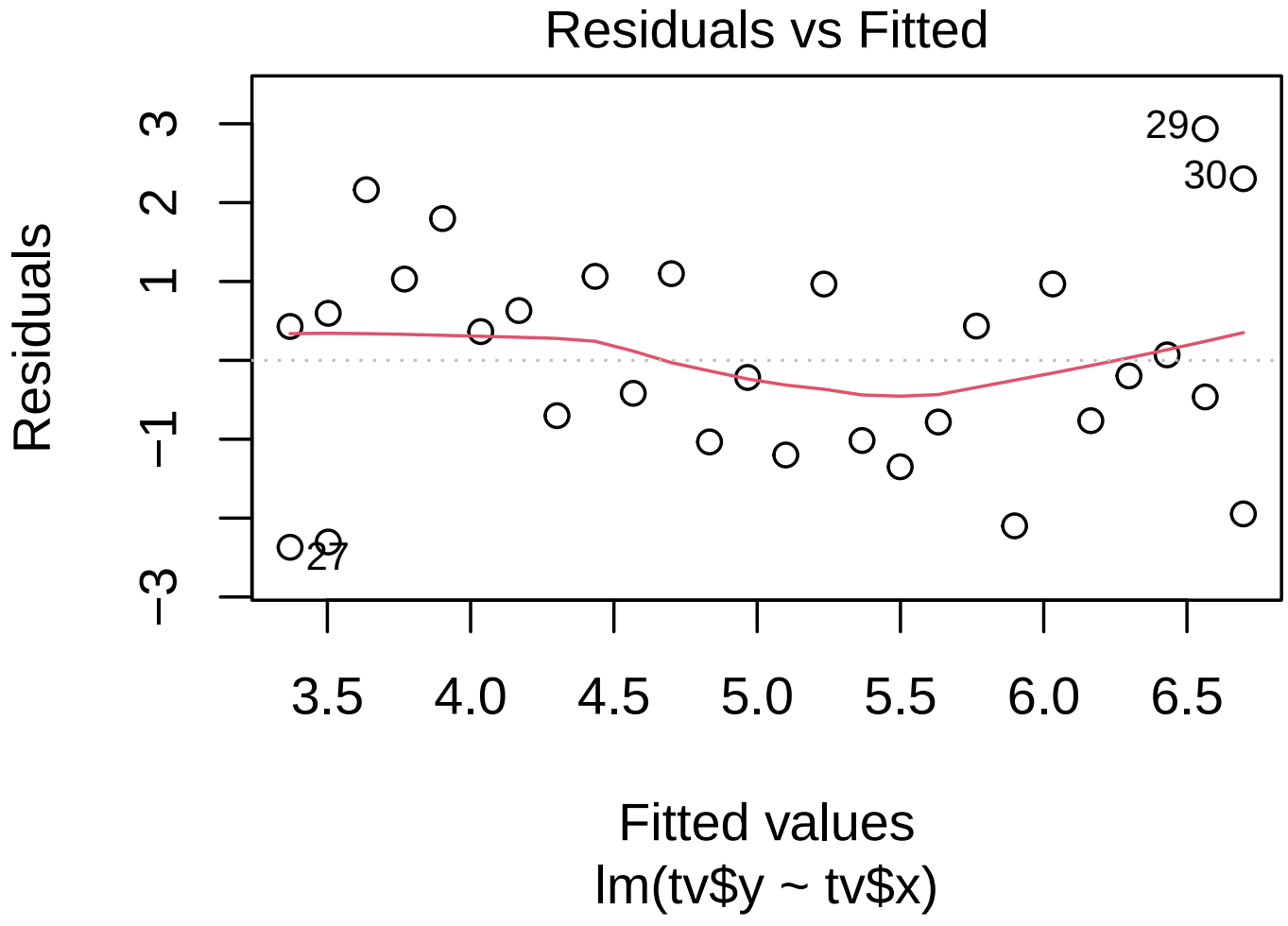
Influential and Atypical Points

```
fittv <- lm(tv$y ~ tv$x)
summary(fittv)
```

```
##
## Call:
## lm(formula = tv$y ~ tv$x)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -2.36994 -0.95755 -0.06405  0.96824  2.93634
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)   1.7065     0.8172   2.088 0.045977 *
## tv$x          0.6654     0.1552   4.287 0.000194 ***
## ---
## Signif. codes:
## 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 1.402 on 28 degrees of freedom
## Multiple R-squared:  0.3963, Adjusted R-squared:  0.3747
## F-statistic: 18.38 on 1 and 28 DF,  p-value: 0.0001939
```

Influential and Atypical Points

```
plot(fittv, which=1)
```

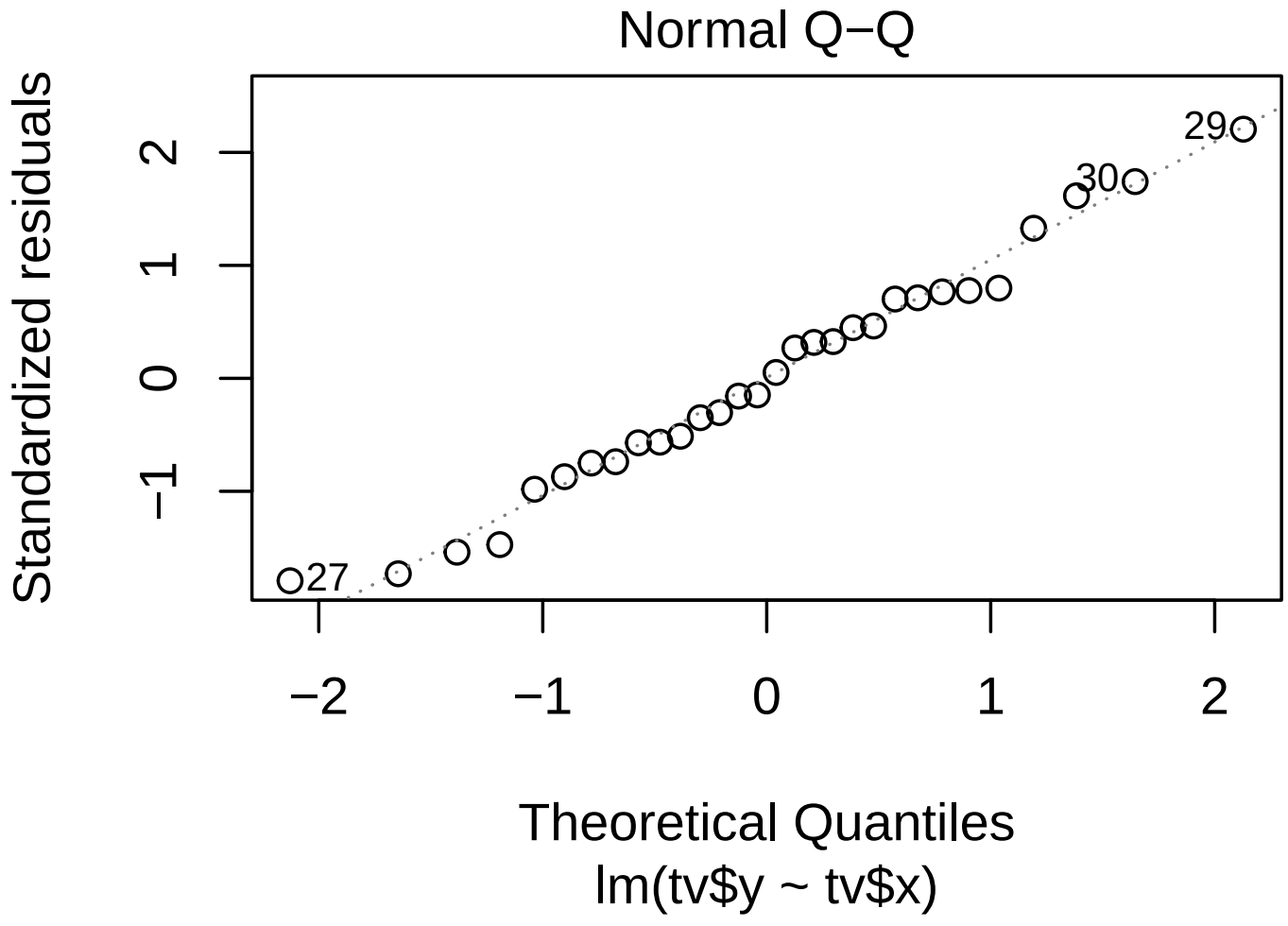


In this plot, we see that there are four points, two on the upper right-hand corner with numbers 29 and 30, and two on the lower left-hand corner, one of which is numbered 27, which seem to 'tilt' the graph because the rest of the points seem to follow a decreasing pattern with a small negative slope.

Next, we plot the other three diagnostic graphs we have considered before.

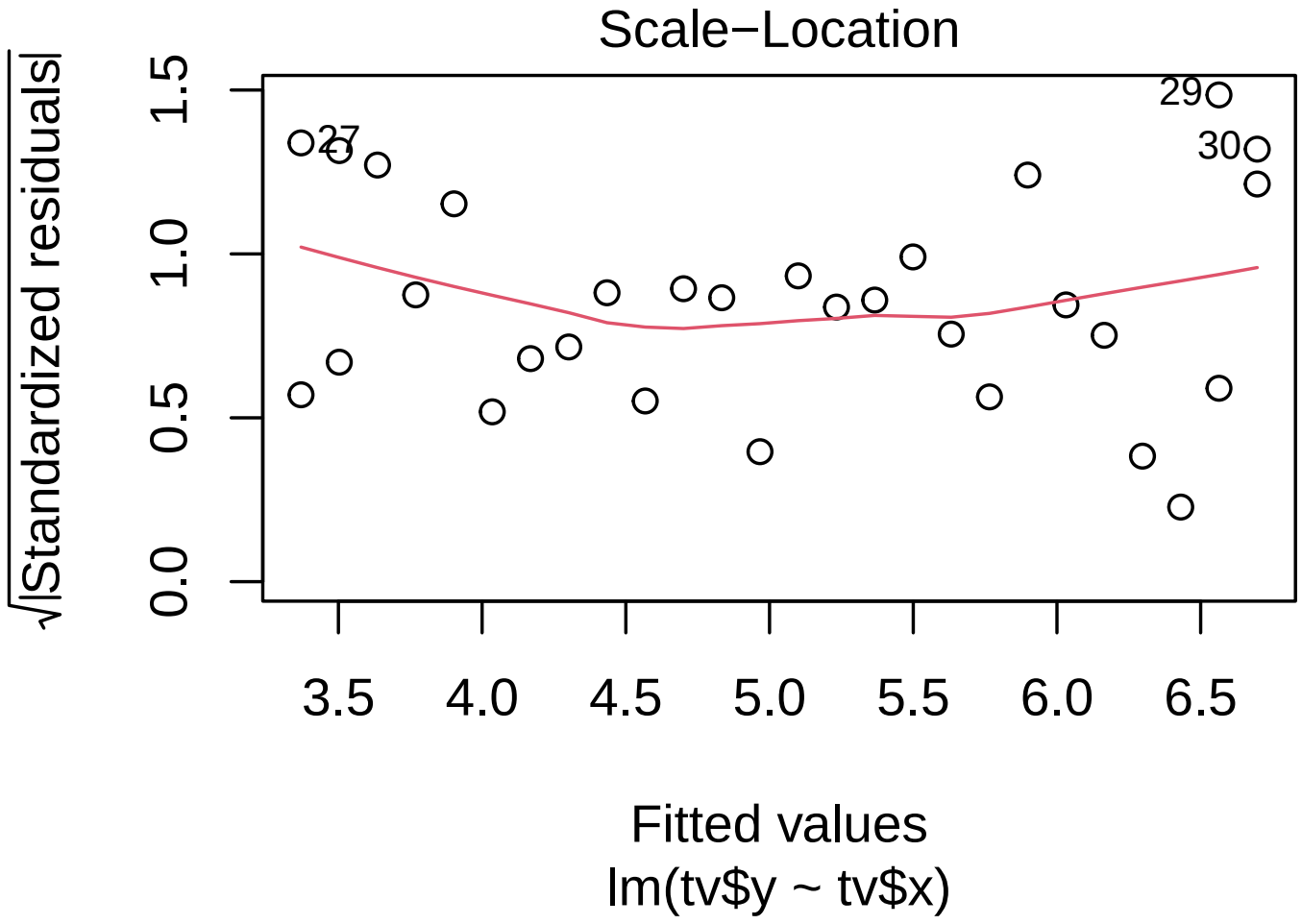
Influential and Atypical Points

```
plot(fittv, which=2)
```



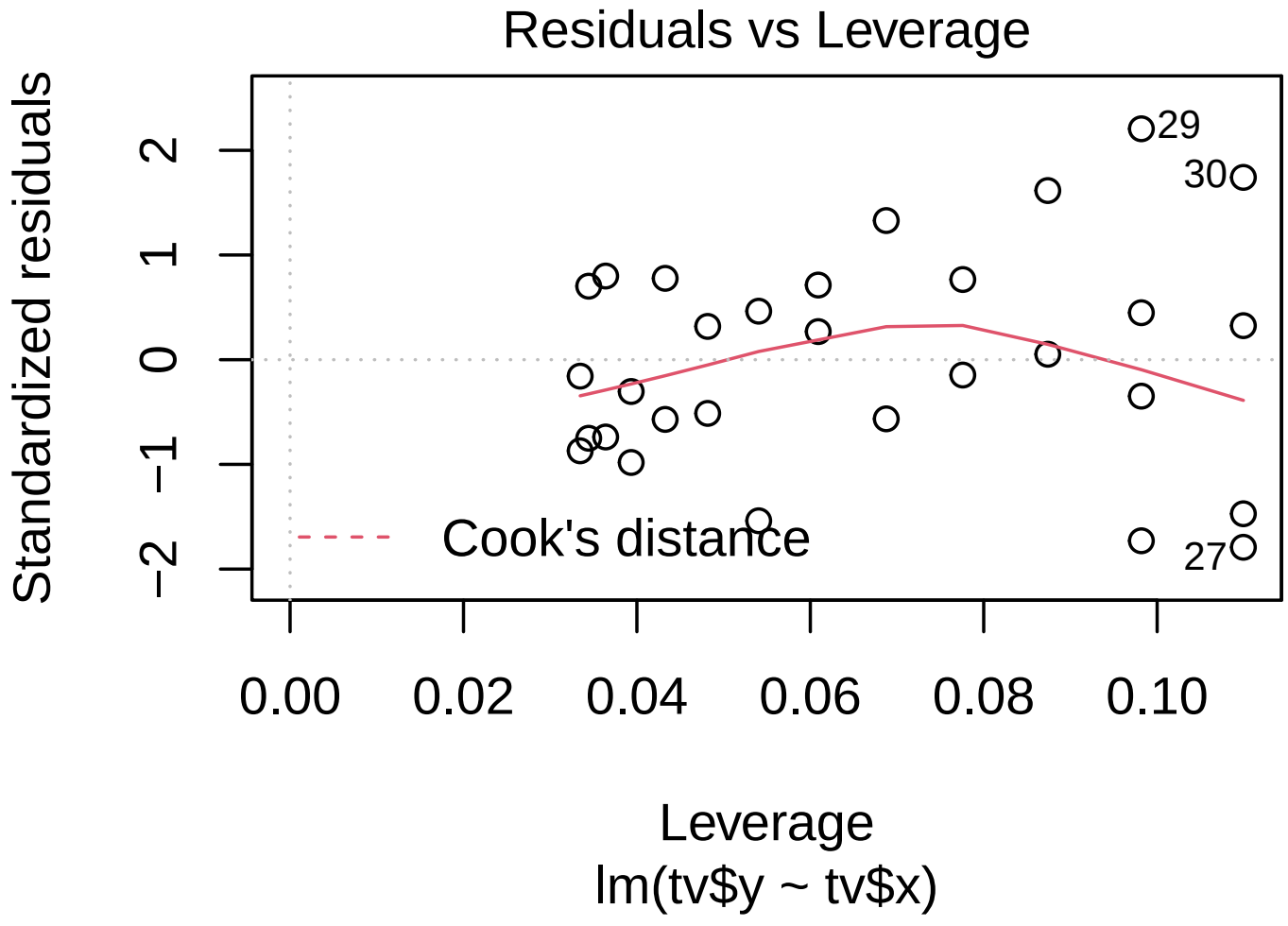
Influential and Atypical Points

```
plot(fittv, which=3)
```



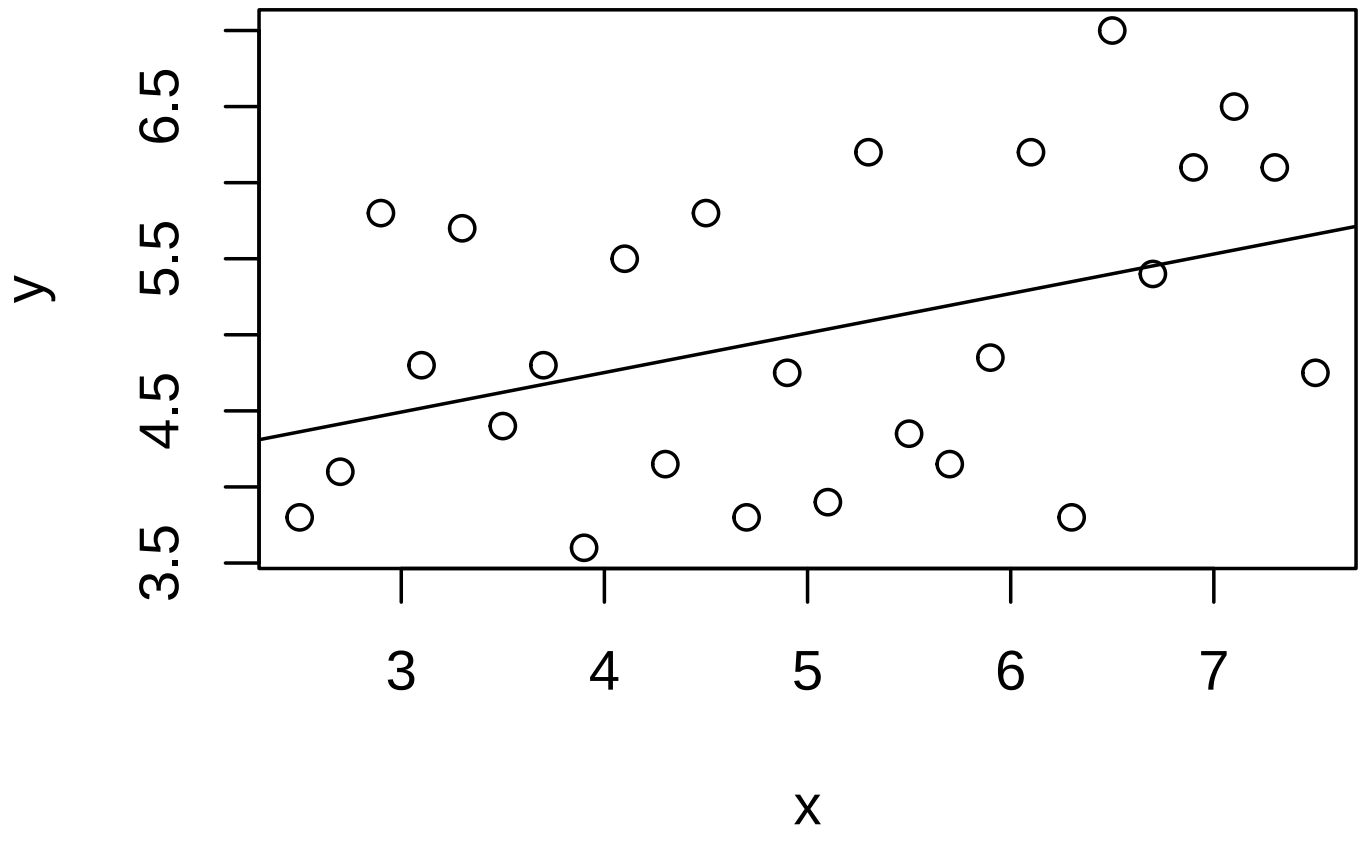
Influential and Atypical Points

```
plot(fittv, which=5)
```



As an exercise we fit the model excluding these four points.

```
tv2 <- tv[1:26,]; plot(tv2)
fittv2 <- lm(tv2$y ~ tv2$x)
abline(fittv2)
```



Influential and Atypical Points

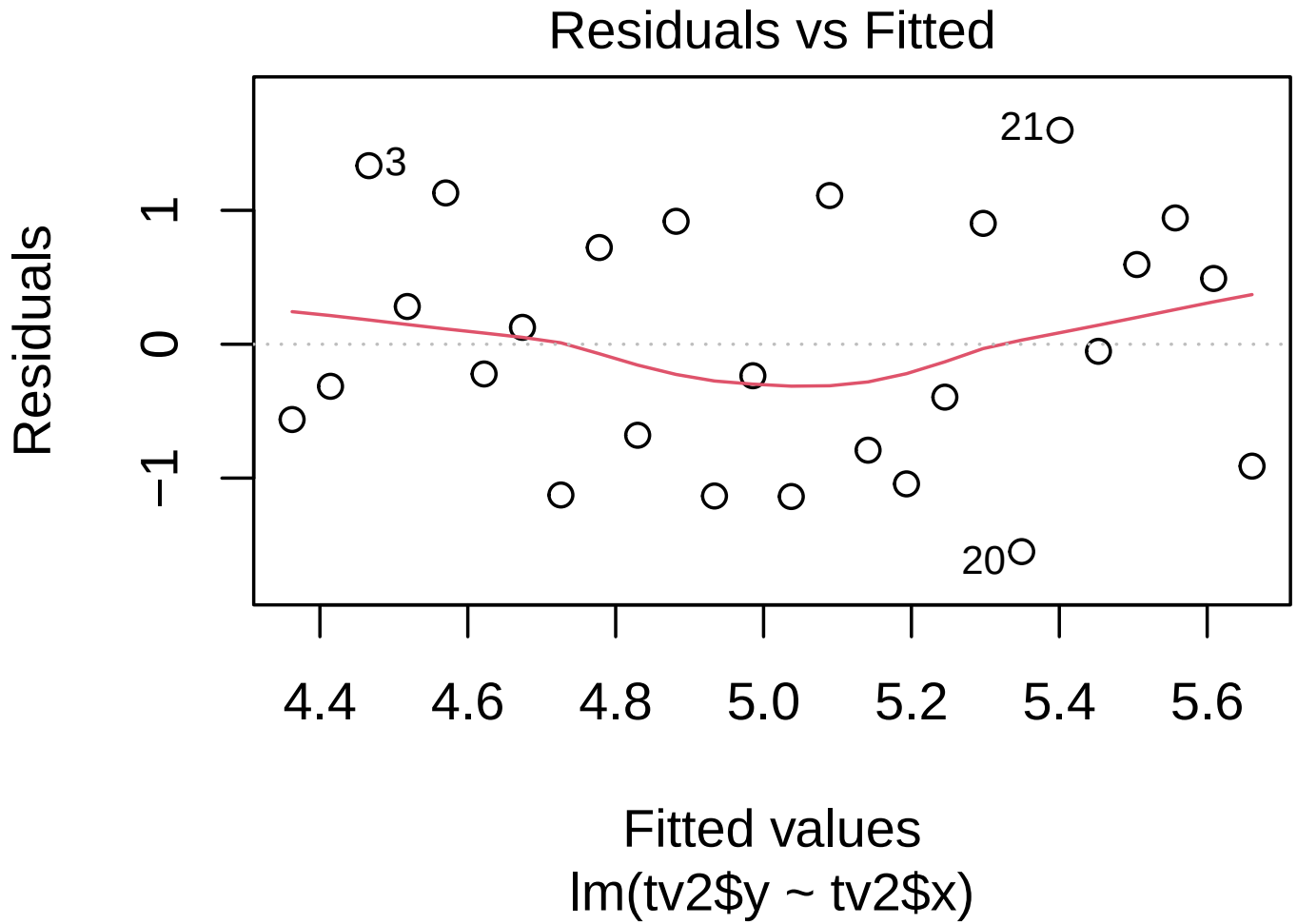
```
summary(fittv2)
```

```
##
## Call:
## lm(formula = tv2$y ~ tv2$x)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -1.5491 -0.7635 -0.1375  0.8577  1.5990
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)   3.7132     0.6314   5.881 4.56e-06 ***
## tv2$x         0.2597     0.1209   2.147   0.0421 *
## ---
## Signif. codes:
## 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.9251 on 24 degrees of freedom
## Multiple R-squared:  0.1611, Adjusted R-squared:  0.1262
## F-statistic: 4.609 on 1 and 24 DF,  p-value: 0.04211
```

Influential and Atypical Points

The results change radically. The slope, which is reduced to 0.26, is moderately significant, and the R^2 goes down to 0.1611.

```
plot(fittv2)
```



Transformed Data

Transformed Data

The data in the `Bacteria` file represent the number (in hundreds) of marine bacteria that survived 200 kilovolt X-ray exposure for periods ranging from 1 to 15 6-minute intervals.

The experiment was conducted to test the hypothesis that bacterial deaths occur when their 'vital center' is struck by a ray. This type of bacteria does not form groups or chains, so the number of bacteria can be estimated by plate counts.

If the theory is correct, the logarithm of the number of survivors must have a linear relationship to the length of the exposure.

If n_t represents the number of surviving bacteria at time t

$$n_t = n_0 e^{\beta t}, \quad t > 0,$$

where n_0 and β are the model parameters and have simple interpretations: n_0 is the number of bacteria at the beginning of the experiment, and β is the rate of destruction or death of the bacteria. Taking logarithms

$$\log n_t = \log n_0 + \beta t = \alpha + \beta t$$

where $\alpha = \log n_0$, and we see that this is a linear function of t. If we add a random error to the model, we get

$$\log n_t = \alpha + \beta t + \epsilon_t$$

and we can now fit a regression model.

If we go back to the original (exponential) model the error appears multiplicatively:

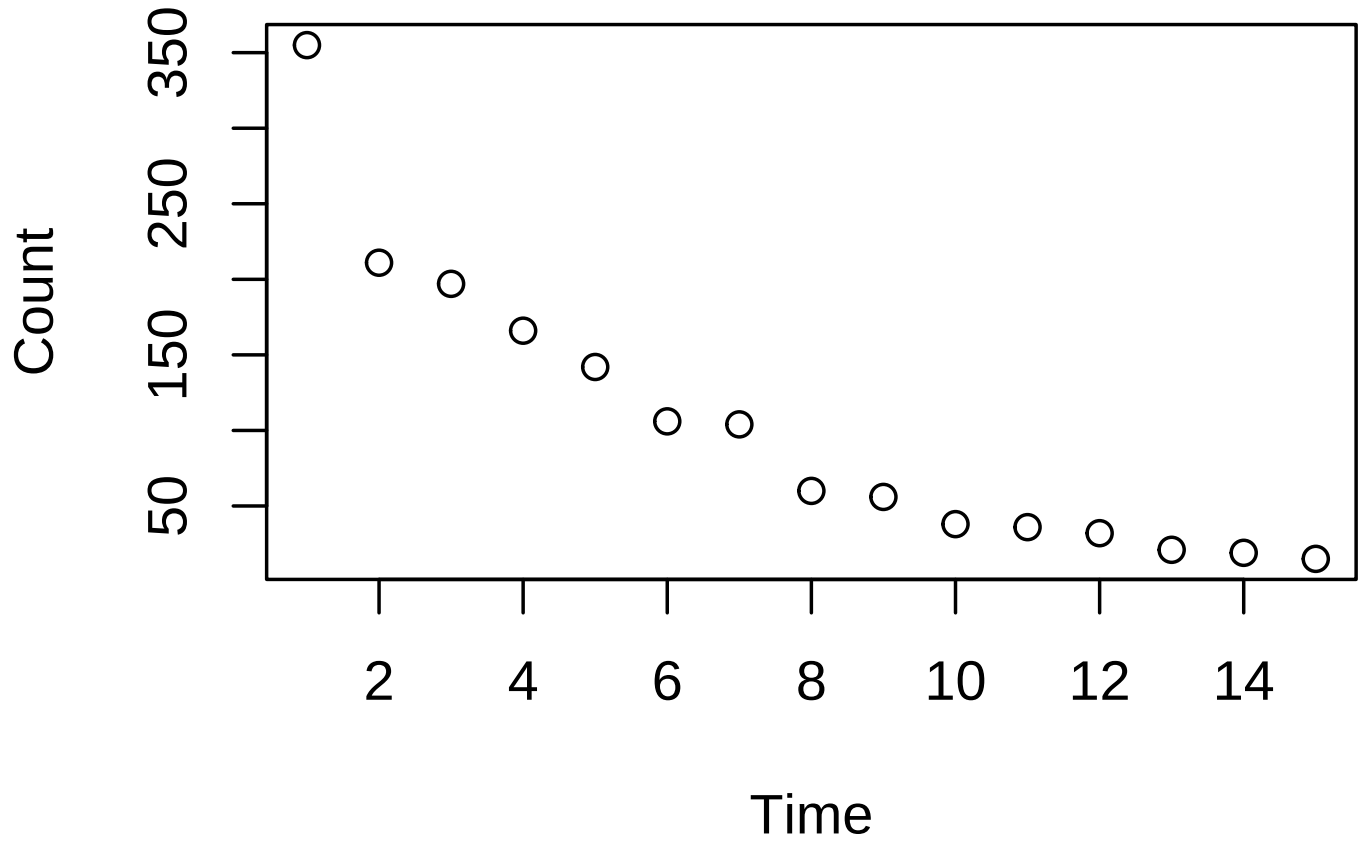
$$n_t = n_0 e^{\beta t} u_t,$$

where $u_t = e^{\epsilon_t}$ is a multiplicative error.

The model assumes that $\epsilon_t = \log u_t$ has a normal distribution and therefore u_t must have lognormal distribution.

We start graphing the data

```
Bacteria <- read.csv('Bacteria.csv')
plot(Bacteria)
```



The graph suggests a non-linear relationship between the two variables.

However, we proceed to fit a linear model to study the consequences. The model is

$$n_t = \alpha + \beta t + \epsilon_t,$$

Transformed Data

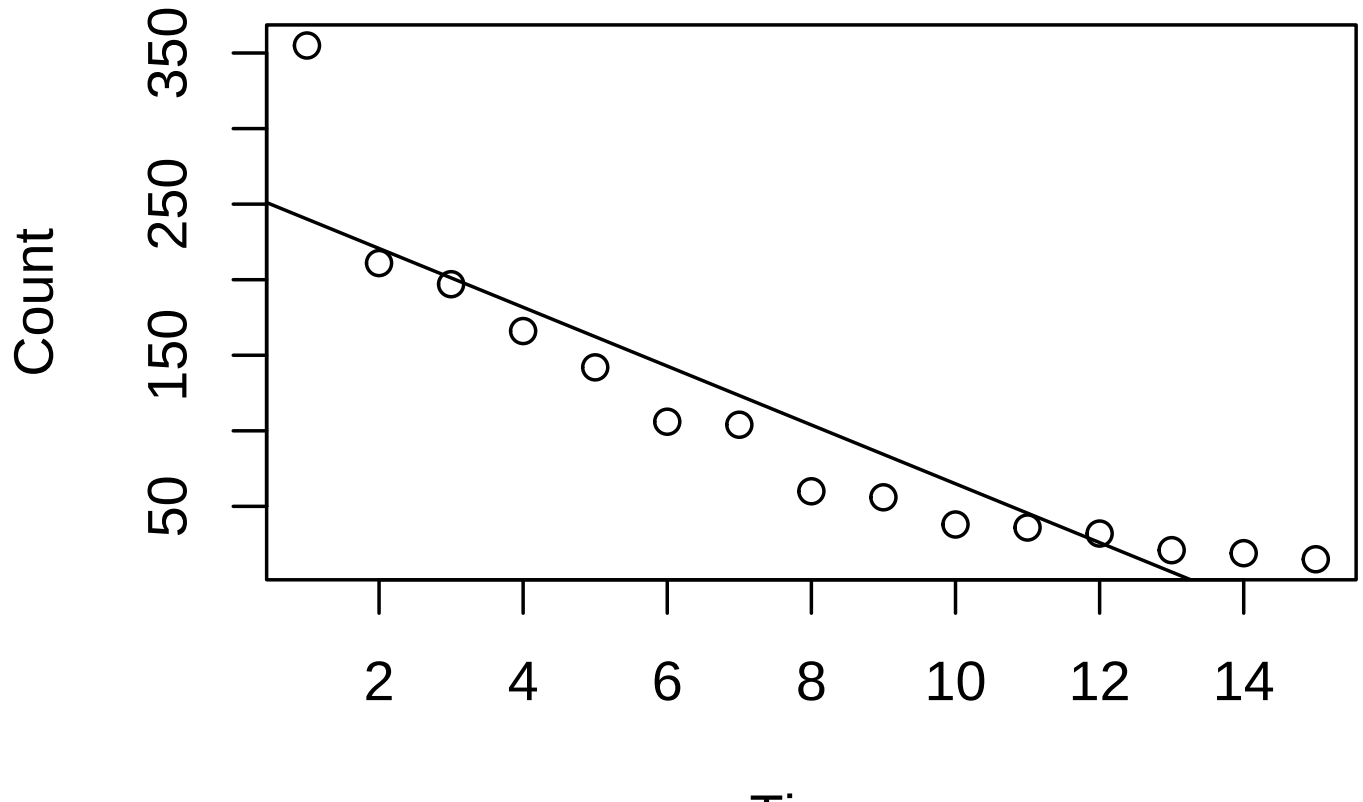
```
attach(Bacteria)
fitbac <- lm(Count ~ Time)
summary(fitbac)
```

```
##
## Call:
## lm(formula = Count ~ Time)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -43.867 -23.599  -9.652  10.223 114.883
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)   259.58      22.73  11.420 3.78e-08 ***
## Time          -19.46       2.50  -7.786 3.01e-06 ***
## ---
## Signif. codes:
## 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 41.83 on 13 degrees of freedom
## Multiple R-squared:  0.8234, Adjusted R-squared:  0.8098
## F-statistic: 60.62 on 1 and 13 DF,  p-value: 3.006e-06
```

Transformed Data

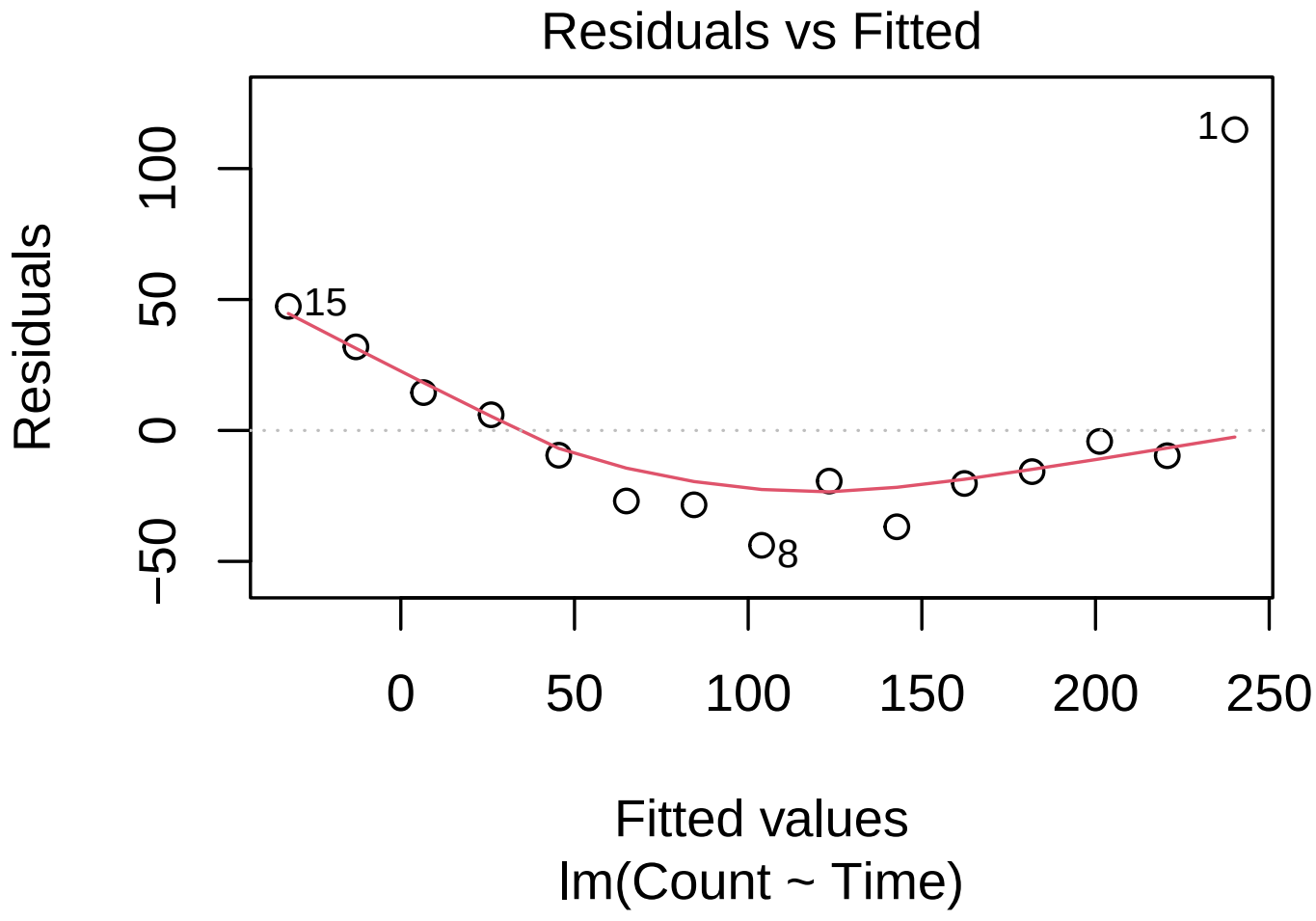
Although the regression coefficient is significant, and we have a high value for R^2, the linear model is not appropriate. A first indication comes from the graph we made, which we repeat adding the regression line

```
plot(Bacteria)
abline(fitbac)
```



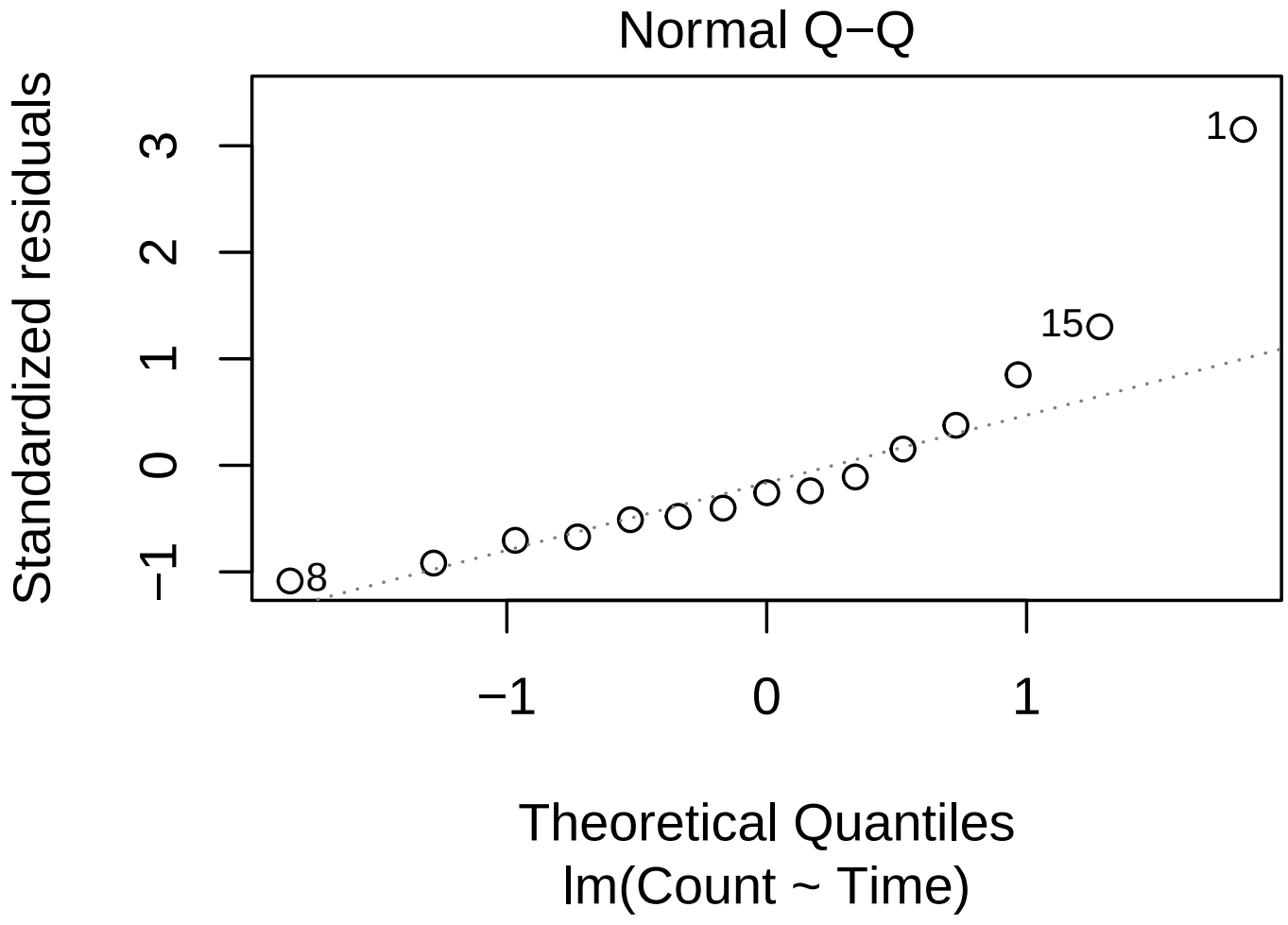
We find more evidence of this in the residuals graphs:

```
plot(fitbac, which=1)
```



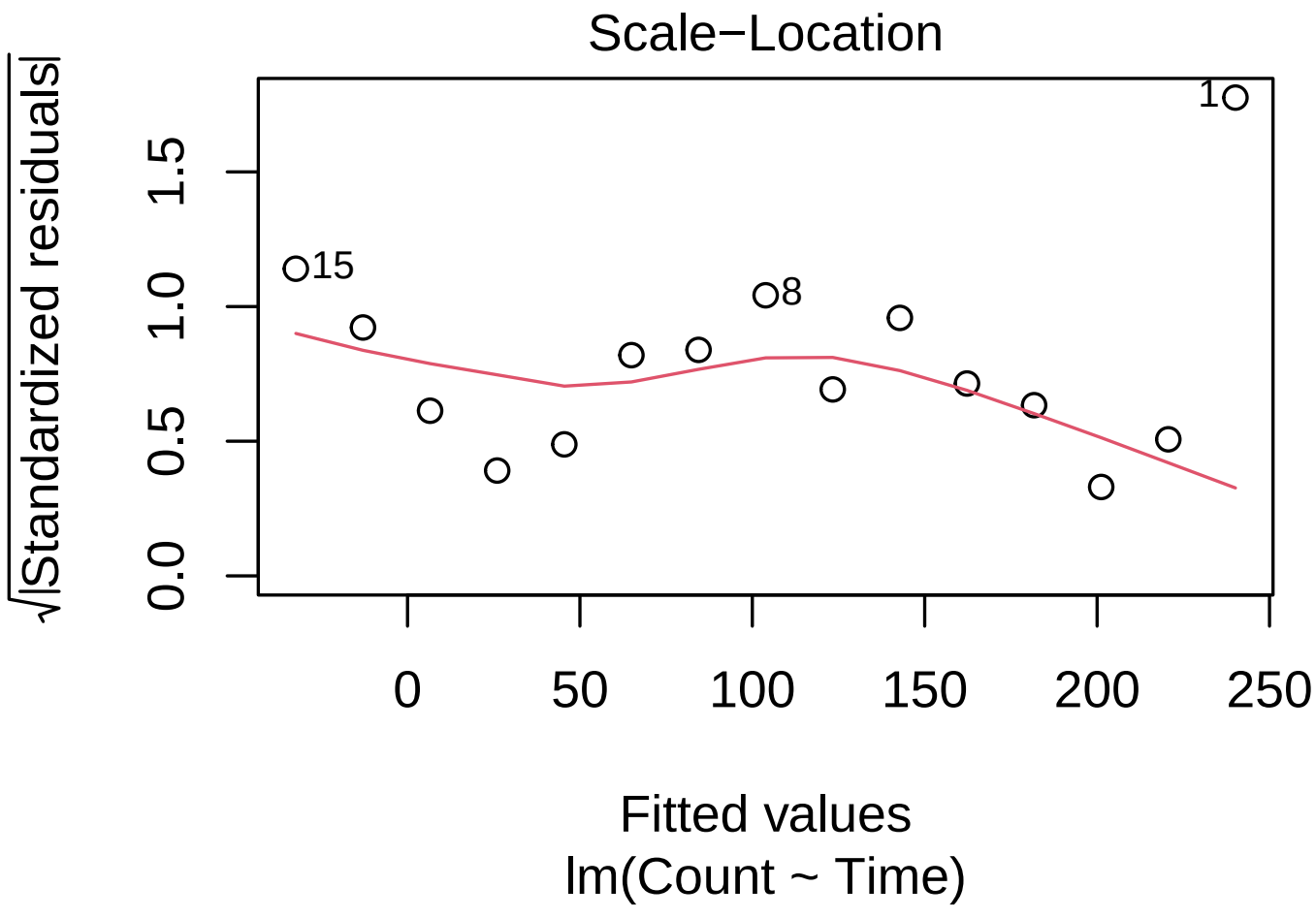
We find more evidence of this in the residuals graphs:

```
plot(fitbac, which=2)
```



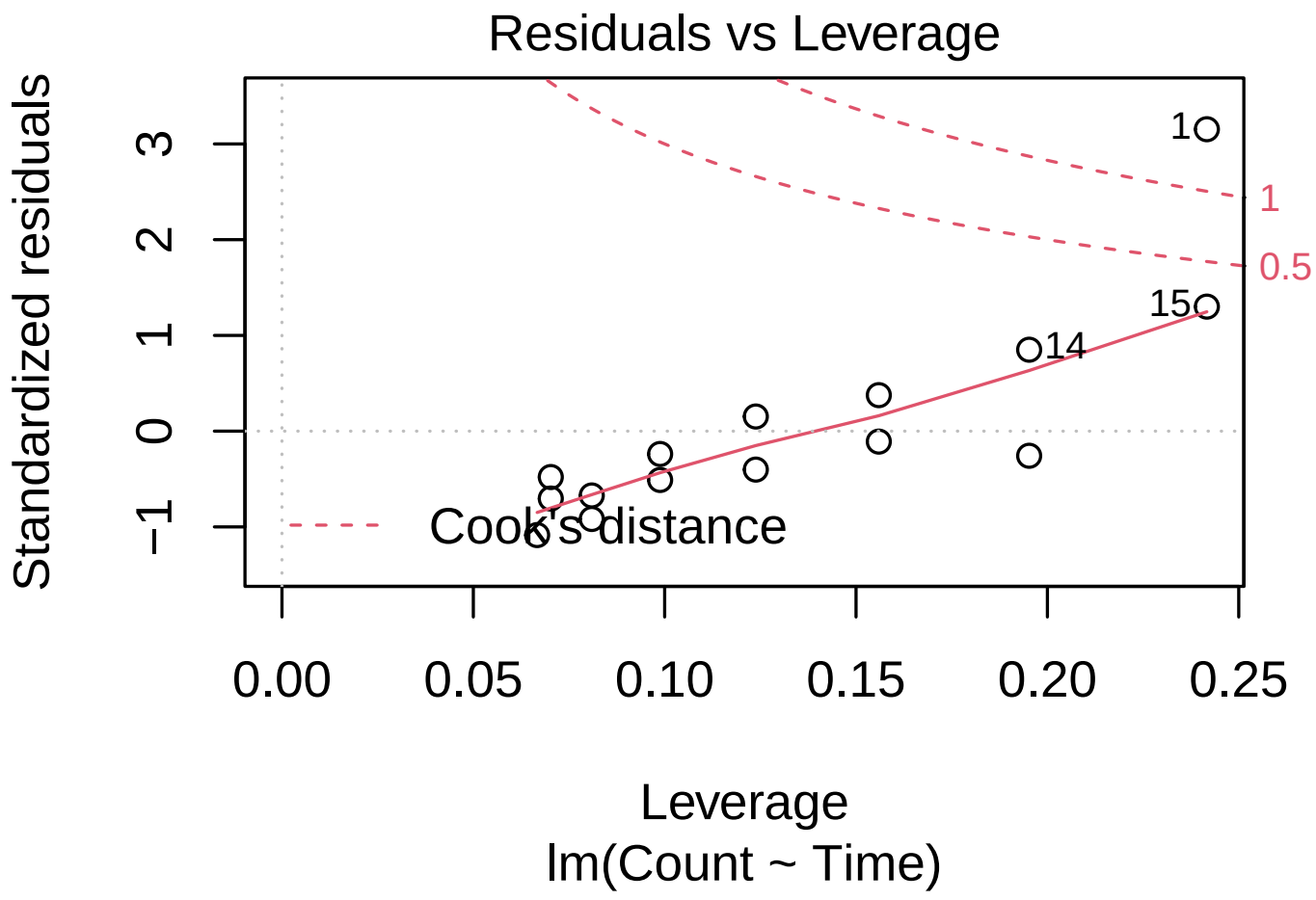
We find more evidence of this in the residuals graphs:

```
plot(fitbac, which=3)
```



We find more evidence of this in the residuals graphs:

```
plot(fitbac, which=5)
```



Transformed Data

The first graph, residuals vs. fitted values, shows that this model does not explain all the relation existing between these two variables.

The quantile plot shows disagreement on the right tail of the distribution.

The third graph shows again that there is a structure in the residuals that has not been included in the model.

Finally, the last graph shows that there are some highly influential points in the regression.

Transformed Data

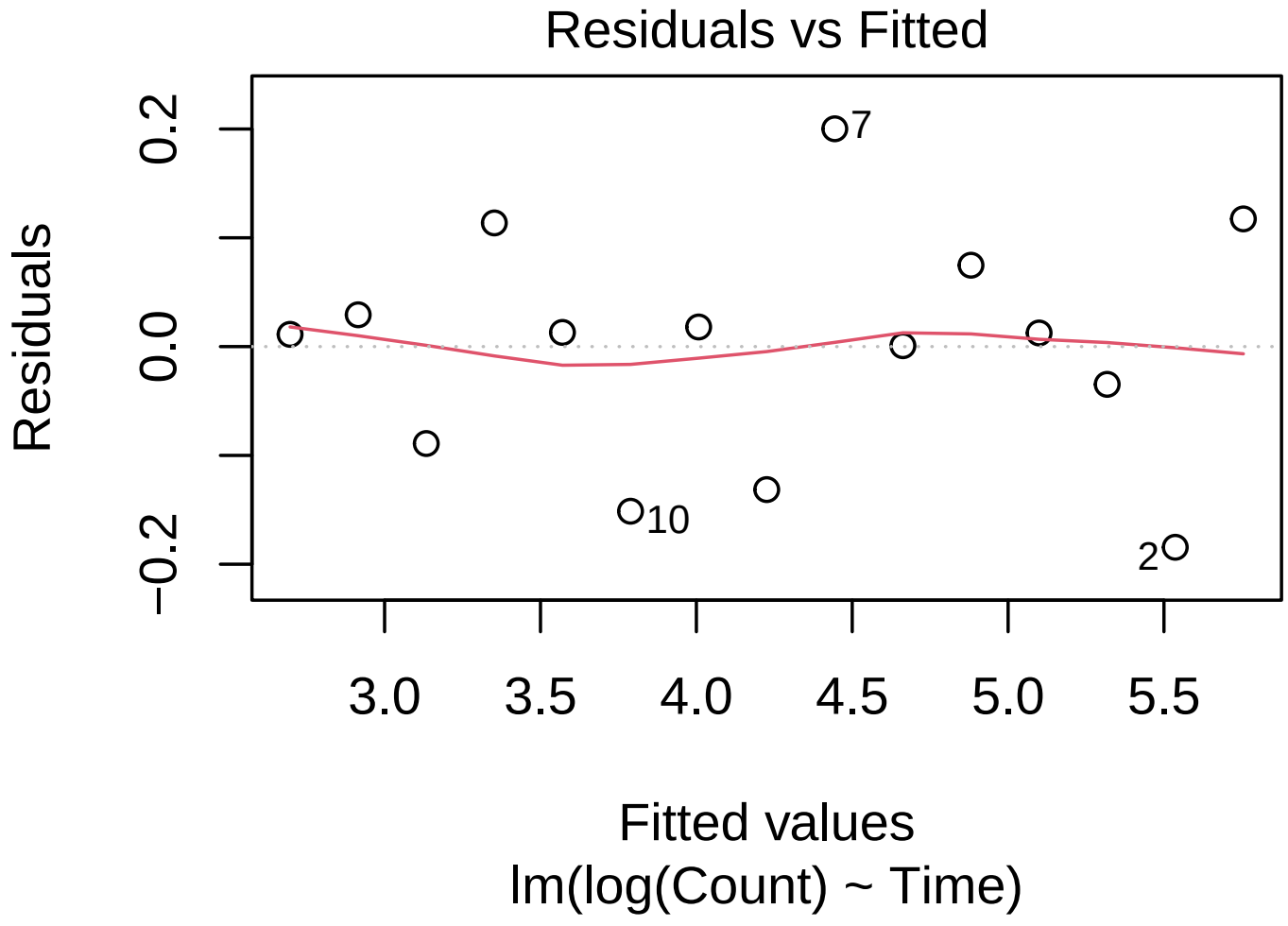
Let's look now at the model using a logarithmic transformation

```
fitlogbac <- lm(log(Count) ~ Time)
summary(fitlogbac)
```

```
##
## Call:
## lm(formula = log(Count) ~ Time)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -0.18445 -0.06189  0.01253  0.05201  0.20021
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)  5.973160   0.059778   99.92  < 2e-16 ***
## Time        -0.218425   0.006575  -33.22 5.86e-14 ***
## ---
## Signif. codes:
## 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.11 on 13 degrees of freedom
## Multiple R-squared:  0.9884, Adjusted R-squared:  0.9875
## F-statistic:  1104 on 1 and 13 DF,  p-value: 5.86e-14
```

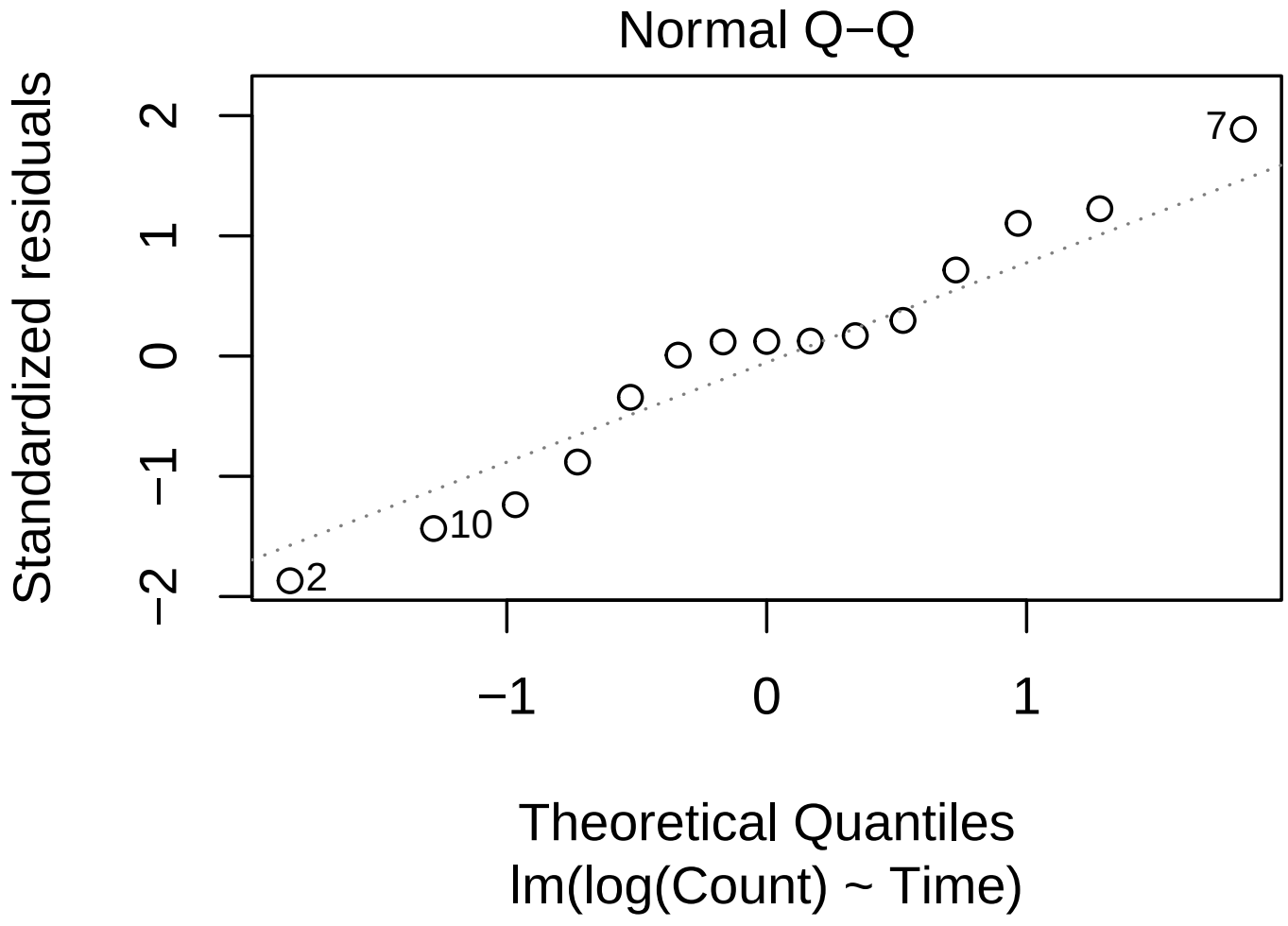
Transformed Data

```
plot(fitlogbac, which=1)
```



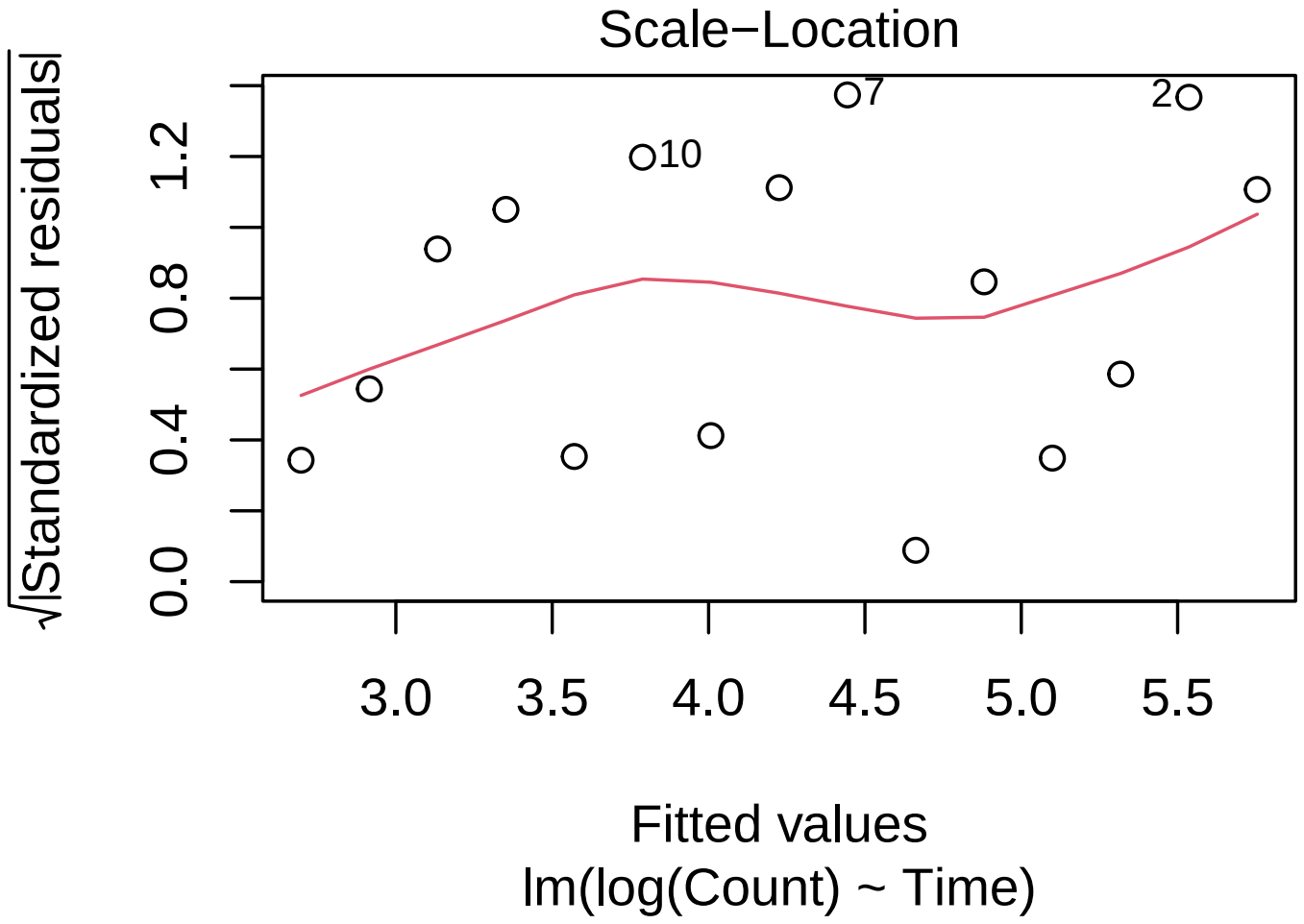
Transformed Data

```
plot(fitlogbac, which=2)
```



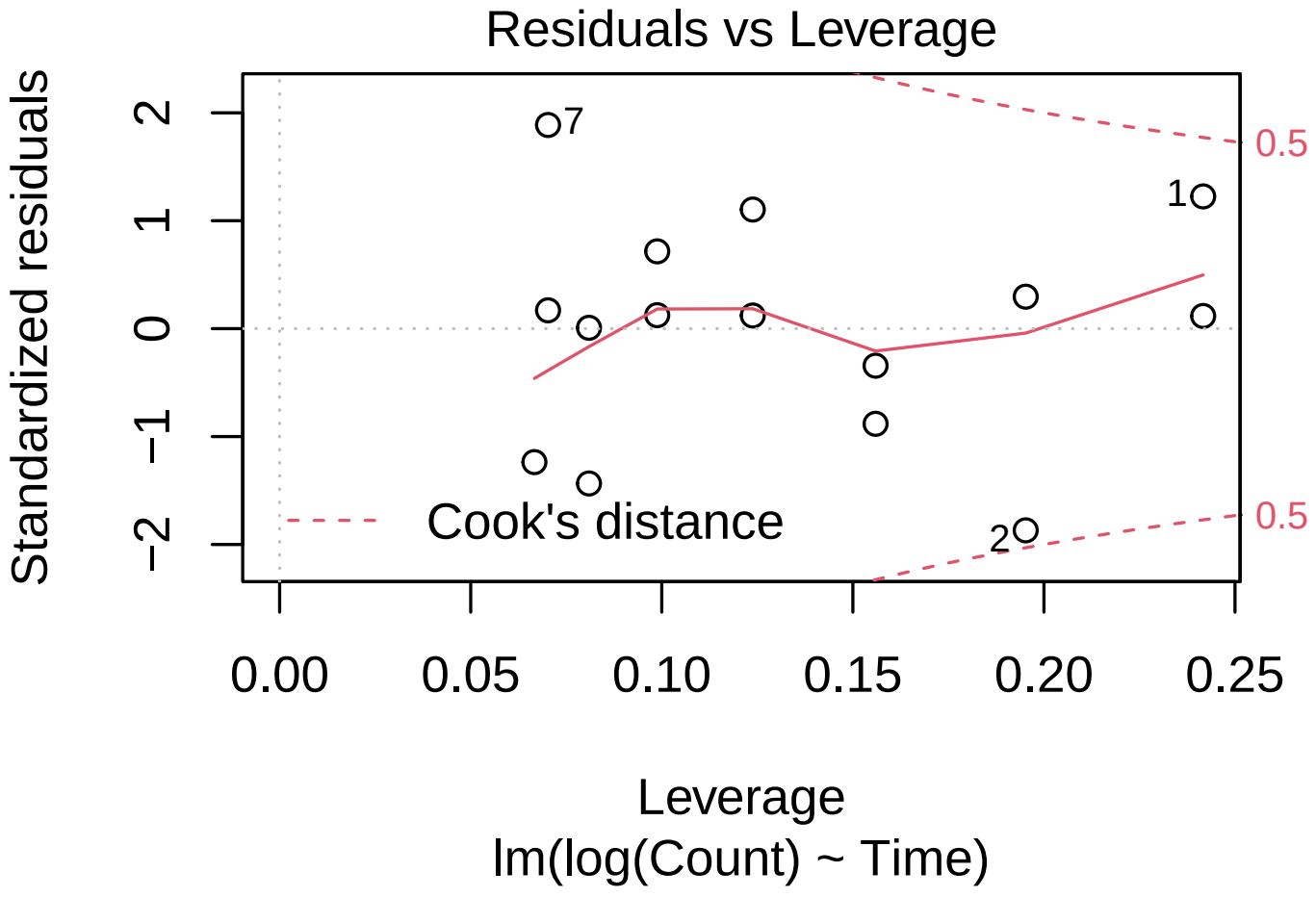
Transformed Data

```
plot(fitlogbac, which=3)
```



Transformed Data

```
plot(fitlogbac, which=5)
```



Transformed Data

We now see that the regression coefficients are significant, standard errors are reasonable, and the model explains about 98% of the variation in the data.

The residual graphs also show a considerably improved fit.

The residuals appear to be randomly distributed, the fit of the experimental data and model predictions is good, and the dispersion of the residuals has been considerably reduced.

The only graph that is not entirely satisfactory is the normal qq-plot, but this may be because we have little data.

The linear model for $log(Count)$ is

$$\log(Count) = 5.97 - 0.219 \cdot t$$

where t is time, and the exponential model is

$$Count = e^{5.97 - 0.219 \cdot t} = 392.75 e^{-0.219 \cdot t}$$