Modelling with R

A Solution to *Two Non-linear Regressions Examples*

1. The data set in the file `rat_data.csv` gives the production of insulin in experimental animals, (rats), in response to a mixture of two drugs. The drug doses are in variables `x1` and `x1`, and the response, in suitable units, is in `y`. The data set comes originally from a paper by Darby and Ellis (1976), *Applied Statistics*, **25**: 298-299.

   A non-linear regression model of the following form has been suggested:

$$y = \alpha + \delta \log\left(x_1 + \rho x_2 + \kappa\sqrt{\rho x_1 x_2}\right) + \epsilon, \qquad \epsilon \sim \mathrm{N}(0, \sigma^2)$$

   Some experimentation has suggested that suitable starting values could be

$$\alpha = -17, \quad \delta = 10, \quad \rho = 0.05, \quad \kappa = -0.03$$

   - Fit the non-linear regression and examine the fit of the model.

     A solution:

```
> rats <- read.csv("rat_data.csv")
> rats.m1 <-
      nls(y ~ alpha + delta*log(x1 + rho*x2 + kappa*sqrt(rho*x1*x2)),
        data = rats, start = c(alpha = -17, delta = 10, rho = 0.05,
                               kappa = -0.03), trace = TRUE)
```

```
251.5351 :  -17.00  10.00   0.05  -0.03
222.2368 :  -17.19756153  10.51979811   0.04567634  -0.34219527
220.1831 :  -17.3652209  10.5447925   0.0465178  -0.2995751
220.1822 :  -17.34135194  10.54000375   0.04649095  -0.30089423
220.1822 :  -17.3421131  10.5401476   0.0464922  -0.3008427
```

```
> summary(rats.m1)
```

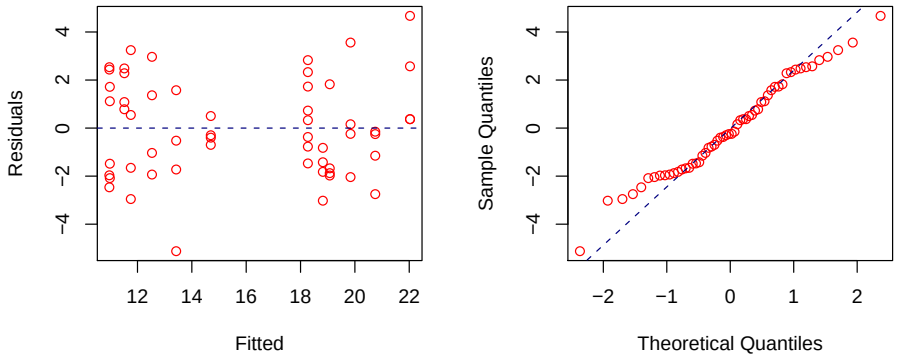
```
Formula: y ~ alpha + delta * log(x1 + rho * x2 + kappa * sqrt(rho * x1 *
    x2))

Parameters:
       Estimate Std. Error t value Pr(>|t|)
alpha -17.342113   2.737099  -6.336 5.65e-08
delta  10.540148   0.792484  13.300  < 2e-16
rho     0.046492   0.003263  14.250  < 2e-16
kappa  -0.300843   0.120408  -2.499   0.0157

Residual standard error: 2.058 on 52 degrees of freedom

Number of iterations to convergence: 4
Achieved convergence tolerance: 3.356e-06
```

```
> rs <- resid(rats.m1)
> fv <- fitted(rats.m1)
> par(mfrow=c(1,2))
> plot(fv, rs, xlab = 'Fitted', ylab = 'Residuals', col = 'red')
> abline(h = 0, col = 'navy', lty = 'dashed')
> qqnorm(rs, main = '', col = 'red')
> qqline(rs, col = 'navy', lty = 'dashed')
```



These diagnostics give no cause to distrust the model.

- Give the parameter estimates and their standard errors.
  See output above.
- Fit the model in the alternative form

$$y = \alpha + \delta \log\left(x_1 + \rho x_2 + \kappa\sqrt{x_1 x_2}\right) + \epsilon, \qquad \epsilon \sim \mathrm{N}(0, \sigma^2)$$

  and explain how the parameter estimates are related.
  A solution would be:

```
> b1 <- coef(rats.m1)
> rats.m2 <-
      nls(y ~ alpha + delta*log(x1 + rho*x2 + kappa*sqrt(x1*x2)),
        data = rats, start = b1, trace = TRUE)
2627.149 :  -17.3421131  10.5401476   0.0464922  -0.3008427
384.0291 :  -16.10914790  10.30901356   0.04676449  -0.16583131
222.4324 :  -17.47787885  10.57709815   0.04689004  -0.07635055
220.1838 :  -17.35920238  10.54367432   0.04654751  -0.06503484
220.1822 :  -17.34183141  10.54010863   0.04649287  -0.06488310
220.1822 :  -17.34210269  10.54014612   0.04649222  -0.06486837
> summary(rats.m2)
Formula: y ~ alpha + delta * log(x1 + rho * x2 + kappa * sqrt(x1 * x2))

Parameters:
        Estimate Std. Error t value Pr(>|t|)
alpha -17.342103   2.737100  -6.336 5.65e-08
delta  10.540146   0.792484  13.300  < 2e-16
rho     0.046492   0.003263  14.250  < 2e-16
kappa  -0.064868   0.025993  -2.496   0.0158

Residual standard error: 2.058 on 52 degrees of freedom

Number of iterations to convergence: 5
Achieved convergence tolerance: 2.851e-06
> b2 <- coef(rats.m2)
> c(b2["kappa"], b1["kappa"]*sqrt(b1["rho"]))
      kappa       kappa
-0.06486837 -0.06486784
```

The relationship is, using an obvious notation, $\kappa_2 = \kappa_1 * \sqrt{\rho_1}$. In the second form the meaning of the κ parameter has changed relative to the first in this way.

2. The data set in the file `bean_data.csv` relates to the growth of an experimental bean plants. The data originally comes from the book *Nonlinear regression modelling: a unified practical approach* (1983). Marcel Decker, by David A. Ratkowsky.

   The variable `y` gives the length of the plant after a fixed growth time and the variable `x` the amount of water supplied.

   Two possible non-linear regression models would be

$$\text{Gompertz}: \quad y = \alpha \exp\left(-\beta\gamma^x\right) + \epsilon$$

$$\text{Logistic}: \quad y = \frac{\alpha}{1 + \exp\left\{-(x-\beta)/\gamma\right\}}$$

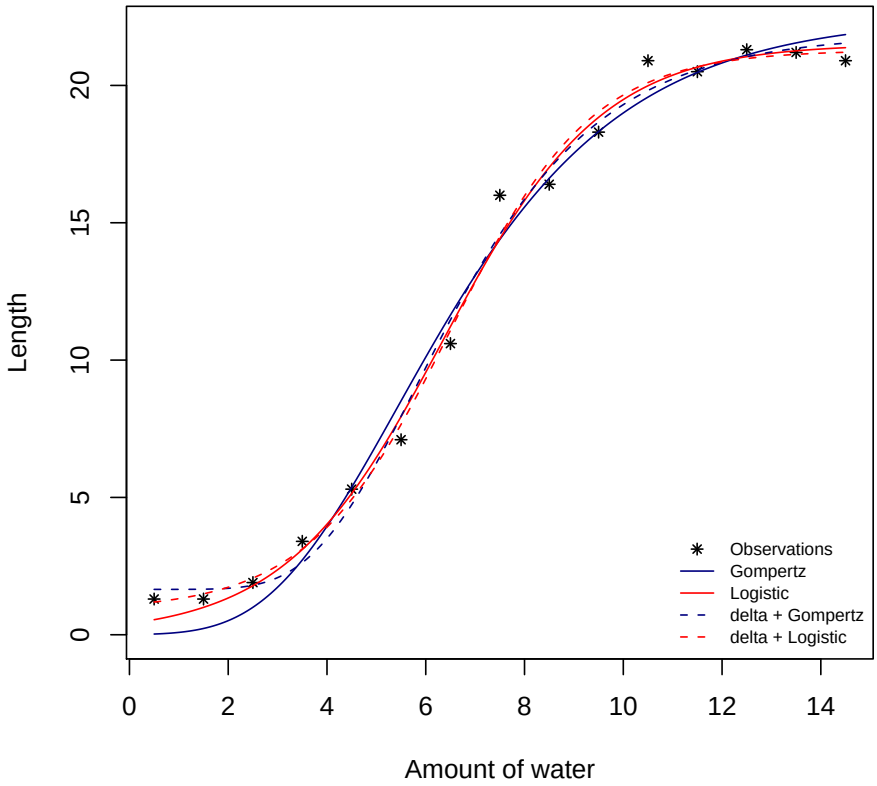
   Self-starting regressin functions are available for both models, namely `SSgompertz` and `SSlogis` in the `stats` package, (which is attached by default).

   - Plot the data.
   - Fit both models and superimpose the fitted lines on the data points in two different colours.

     A solution to both parts above is as follows:

```
> feijao <- read.csv("bean_data.csv")
> with(feijao, plot(x, y, pch=8, cex = 0.7, xlab = "Amount of water",
                    ylab = "Length", ylim = c(0,22)))
> pFei <- with(feijao, data.frame(x = seq(min(x), max(x), len = 1000)))
> fei.gz <- nls(y ~ SSgompertz(x, alpha, beta, gamma), feijao)
> fei.lo <- nls(y ~ SSlogis(x, alpha, beta, gamma), feijao)
> pFei.gz <- predict(fei.gz, pFei)
> pFei.lo <- predict(fei.lo, pFei)
> with(pFei, {
      lines(x, pFei.gz, col = "navy")
      lines(x, pFei.lo, col = "red")
   })
> bstart <- c(delta = 0, coef(fei.gz))
> fei.gz1 <- nls(y ~ delta + alpha*exp(-beta*gamma^x),
               data = feijao, start = bstart, trace = TRUE)
12.59049 :   0.0000000 22.5065984  8.2175122  0.6783303
10.80006 :   1.7055933 20.2105212 12.1515046  0.6364683
6.978755 :   1.5897493 20.3686624 14.3455543  0.6300065
6.858026 :   1.627120 20.244532 15.696748  0.621974
6.845719 :   1.6431409 20.2193253 16.0527593  0.6204618
6.845284 :   1.6491437 20.2079042 16.1640857  0.6198634
6.845264 :   1.650654 20.205516 16.187592  0.619743
6.845263 :   1.6509895 20.2049639 16.1928599  0.6197152
6.845263 :   1.6510623 20.2048473 16.1939747  0.6197094
6.845263 :   1.6510779 20.2048222 16.1942139  0.6197081
> bstart <- c(delta = 0, coef(fei.lo))
> fei.lo1 <- nls(y ~ delta + alpha/(1 + exp(-(x - beta)/gamma)),
               data = feijao, start = bstart, trace = TRUE)
```

```
6.210243 :   0.000000 21.508903  6.360354  1.607239
5.20133 :   0.9519087 20.3240469  6.5150838  1.4303138
5.189891 :   0.8844376 20.3987972  6.5012742  1.4332526
5.189891 :   0.8844725 20.3988558  6.5013730  1.4332403
> pFei.gz1 <- predict(fei.gz1, pFei)
> pFei.lo1 <- predict(fei.lo1, pFei)
> with(pFei, {
      lines(x, pFei.gz1, col = "navy", lty = "dashed")
      lines(x, pFei.lo1, col = "red", lty = "dashed")
    })
> legend("bottomright", c("Observations", "Gompertz", "Logistic",
    "delta + Gompertz", "delta + Logistic"),
    pch = c(8, rep(NA, 4)),
    lty = c(NA, rep(c("solid", "dashed"), each = 2)),
    col = c("black", rep(c("navy", "red"), 2)), bty = "n", cex = 0.7)
```



- Extend both models by adding a constant to the model function, say δ.
  Done above.
- In each case, test the model that the additional constant improves the fit.
  A solution is as follows:

```
> anova(fei.gz, fei.gz1)
Analysis of Variance Table

Model 1: y ~ SSgompertz(x, alpha, beta, gamma)
Model 2: y ~ delta + alpha * exp(-beta * gamma^x)
```

```
  Res.Df Res.Sum Sq Df  Sum Sq F value  Pr(>F)
1     12    12.5905
2     11     6.8453  1  5.7452  9.2323 0.01128
```

```
> anova(fei.lo, fei.lo1)
Analysis of Variance Table

Model 1: y ~ SSlogis(x, alpha, beta, gamma)
Model 2: y ~ delta + alpha/(1 + exp(-(x - beta)/gamma))
  Res.Df Res.Sum Sq Df Sum Sq F value Pr(>F)
1     12     6.2102
2     11     5.1899  1 1.0204  2.1626 0.1694
```

In the case of the Gompertz growth model, the fit is significantly improve, but not for the Logistic growt model.

- Add the two lines from the extended models to the plot, using the same colors as before, but a different line type.

  Done above.

- Add a legend to your plot stating what the lines and symbols mean. Place the legend in the lower right-hand corner of the plot.

  Done above.