Using R for Linear Regression

In the following handout words and symbols in **bold** are R functions and words and symbols in *italics* are entries supplied by the user; underlined words and symbols are optional entries (all current as of version R-2.4.1). Sample texts from an R session are highlighted with gray shading.

Suppose we prepare a calibration curve using four external standards and a reference, obtaining the data shown here:

```
> conc
[1] 0  10  20  30  40  50

> signal
[1]  4 22  44  60  82
```

The expected model for the data is

$$\text{signal} = \beta_o + \beta_1 \times \text{conc}$$

where β_o is the theoretical y-intercept and β_1 is the theoretical slope. The goal of a linear regression is to find the best estimates for β_o and β_1 by minimizing the residual error between the experimental and predicted signal. The final model is

$$\text{signal} = b_o + b_1 \times \text{conc} + e$$

where b_o and b_1 are the estimates for β_o and β_1 and e is the residual error.

Defining Models in R

To complete a linear regression using R it is first necessary to understand the syntax for defining models. Let's assume that the dependent variable being modeled is Y and that A, B and C are independent variables that might affect Y. The general format for a linear[1] model is

response ~ op1 term1 op2 term 2 op3 term3…

[1] When discussing models, the term 'linear' does not mean a straight-line. Instead, a linear model contains additive terms, each containing a single multiplicative parameter; thus, the equations

$$y = \beta_0 + \beta_1 x \qquad y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 \qquad y = \beta_0 + \beta_{11} x^2 \qquad y = \beta_0 + \beta_1 x_1 + \beta_2 \log(x_2)$$

are linear models. The equation $y = \alpha x^{\beta}$, however, is not a linear model.

where *term* is an object or a sequence of objects and *op* is an operator, such as a + or a −, that indicates how the term that follows is to be included in the model. The table below provides some useful examples. Note that the mathematical symbols used to define models do not have their normal meanings!

Syntax	Model	Comments
Y ~ A	$Y = \beta_o + \beta_1 A$	Straight-line with an implicit y-intercept
Y ~ -1 + A	$Y = \beta_1 A$	Straight-line with no y-intercept; that is, a fit forced through (0,0)
Y ~ A + I(A^2)	$Y = \beta_o + \beta_1 A + \beta_2 A^2$	Polynomial model; note that the identity function **I( )** allows terms in the model to include normal mathematical symbols.
Y ~ A + B	$Y = \beta_o + \beta_1 A + \beta_2 B$	A first-order model in A and B without interaction terms.
Y ~ A:B	$Y = \beta_o + \beta_1 AB$	A model containing only first-order interactions between A and B.
Y ~ A*B	$Y = \beta_o + \beta_1 A + \beta_2 B + \beta_3 AB$	A full first-order model with a term; an equivalent code is Y ~ A + B + A:B.
Y ~ (A + B + C)^2	$Y = \beta_o + \beta_1 A + \beta_2 B + \beta_3 C + \beta_4 AB + \beta_5 AC + \beta_6 AC$	A model including all first-order effects and interactions up to the n^th order, where n is given by **( )^n**. An equivalent code in this case is Y ~ A*B*C – A:B:C.

Completing a Regression Analysis

The basic syntax for a regression analysis in R is

lm(*Y ~ model***)**

where *Y* is the object containing the dependent variable to be predicted and *model* is the formula for the chosen mathematical model. The command **lm( )** provides the model's coefficients but no further statistical information; thus

```
> lm(signal ~ conc)

Call:
lm(formula = signal ~ conc)

Coefficients:
(Intercept)       conc
 3.60             1.94
```

To obtain more useful information, and to obtain access to many more useful functions for manipulating the data, it is best to create an object that contains the command for the model

```
    > lm.r = lm(signal ~ conc)
```

This object can then be used as an argument for other commands. To obtain a more complete statistical summary of the model, for example, we use the **summary( )** command.

```
  > summary(lm.r)

    Call:
    lm(formula = signal ~ conc)

    Residuals:
      1       2      3      4      5
     0.4   -1.0   1.6   -1.8   0.8

    Coefficients:
                 Estimate Std.  Error     t value    Pr(>|t|)
       (Intercept)  3.60000    1.23288    2.92      0.0615 .
       conc         1.94000    0.05033   38.54   3.84e-05 ***
    ---
    Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

    Residual standard error: 1.592 on 3 degrees of freedom
    Multiple R-Squared: 0.998,      Adjusted R-squared: 0.9973
    F-statistic:  1486 on 1 and 3 DF,  p-value: 3.842e-05
```

The section of output labeled 'Residuals' gives the difference between the experimental and predicted signals. Estimates for the model's coefficients are provided along with the their standard deviations ('Std Error'), and a t-value and probability for a null hypothesis that the coefficients have values of zero. In this case, for example, we see that there is no evidence that the intercept (β_o) is different from zero and strong evidence that the slope (β_1) is significantly different than zero. At the bottom of the table we find the standard deviation about the regression (s_r or residual standard error), the correlation coefficient and an F-test result on the null hypothesis that the MS_{reg}/MS_{res} is 1.

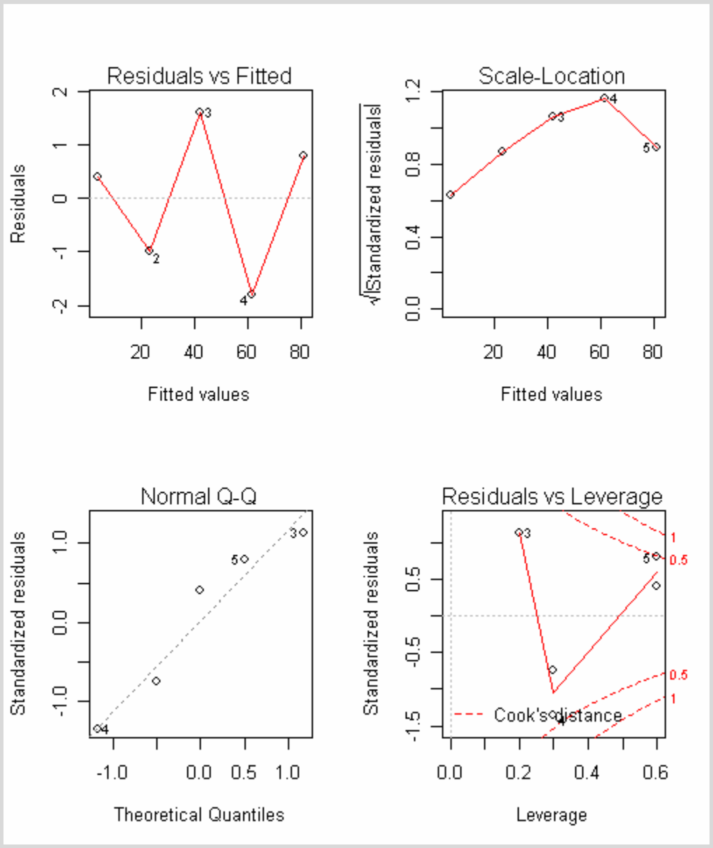
Other useful commands are shown below:

```
    > coef(lm.r)                                      # gives the model's coefficients

    (Intercept)          conc
      3.69               1.94
    > resid(lm.r)                                        # gives the residual errors in Y

       1      2    3      4     5
     0.4   -1.0  1.6   -1.8    0.8

> fitted(lm.r)                                          # gives the predicted values for Y

       1     2         3     4       5
     3.6   23.0   42.4   61.8   81.2
```

Evaluating the Results of a Linear Regression

Before accepting the result of a linear regression it is important to evaluate it suitability at explaining the data. One of the many ways to do this is to visually examine the residuals. If the model is appropriate, then the residual errors should be random and normally distributed. In addition, removing one case should not significantly impact the model's suitability. R provides four graphical approaches for evaluating a model using the **plot( )** command.

```
    > layout(matrix(1:4,2,2))
    > plot(lm.r)
```



The plot in the upper left shows the residual errors plotted versus their fitted values. The residuals should be randomly distributed around the horizontal line representing a residual error of zero; that is, there should not be a distinct trend in the distribution of points. The plot in the lower left is a standard Q-Q plot, which should suggest that the residual errors are normally distributed. The scale-location plot in the upper right shows the square root of the standardized residuals (sort of a square root of relative error) as a function of the fitted values. Again, there should be no obvious trend in this plot. Finally, the plot in the lower right shows each points leverage, which is a measure of its importance in determining the regression result. Superimposed on the plot are contour lines for the Cook's distance, which is another measure of the importance of each observation to the regression. Smaller distances means that removing the observation has little affect on the regression results. Distances larger than 1 are suspicious and suggest the presence of a possible outlier or a poor model.

Sometimes a model has known values for one or more of its parameters. For example, suppose we know that the true model relating the signal and concentration is

$$\text{signal} = 3.00 \times \text{conc}$$

Our regression model is

$$\text{signal} = 3.60 + 1.94 \times \text{conc}$$

We can use a standard t-test to evaluate the slope and intercept. The confidence interval for each is

$$\beta_o = b_o \pm ts_{bo} \qquad \beta_1 = b_1 \pm ts_{b1}$$

where s_{bo} and s_{b1} are the standard errors for the intercept and slope, respectively. To determine if there is a significant difference between the expected (β) and calculated (b) values we calculate t and compare it to its standard value for the correct number of degrees of freedom, which in this case is 3 (see earlier summary).

```
> tb1 = abs((3.00 – 1.94)/0.05033); tb1          # calculate absolute value of t

 [1] 21.06100

> pt(tb1, 3, lower.tail = FALSE)                 # calculate probability for t

[1] 0.0001170821                                 # double this value for a two-
                                                 # tailed evaluation; difference
                                                 # is significant at p = 0.05

> tb0=abs((0-3.60)/1.23288);tb0                  # calculate absolute value of t

[1] 2.919992
```

```
> pt(tb0, 3, lower.tail = FALSE)                 # calculate probability for t

[1] 0.03074826                                   # double this value for a two-
                                                 # tailed evaluation; difference
                                                 # is not significant at p = 0.05
```

Here we calculate the absolute value of t using the calculated values and standard errors from our earlier summary of results. The command

pt(*value, degrees of freedom,* **lower.tail = FALSE)**

returns the one-tailed probability that there is no difference between the expected and calculated values. In this example, we see that there is evidence that the calculated slope of 1.94 is significantly different than the expected value of 3.00. The expected intercept of 0, however, is not significantly different than the calculated value of 3.60. Note that the larger standard deviation for the intercept makes it more difficult to show that there is a significant difference between the experimental and theoretical values.

Using the Results of a Regression to Make Predictions

The purpose of a regression analysis, of course, is to develop a model that can be used to predict the results of future experiments. In our example, for instance, the calibration equation

signal = 3.60 + 1.94×conc

Because there is uncertainty in both the calculated slope and intercept, there will be uncertainty in the calculated signals.

Suppose we wish to predict the signal for concentrations of 0.05, 0.15, 0.25, 0.35 and 0.45 along with the confidence interval for each We can use the **predict( )** command to do this; the syntax is

predict(*model,* **data.frame(***pred = new pred***)**, *level = 0.95*, *interval = "confidence"***)**

where *pred* is the object containing the original independent variables and *new pred* is the object containing the new values for which predictions are desired, and *level* is the desired confidence level.

```
> newconc=c(5,15,25,35,45);newconc

 [1] 5 15  25  35  45

> predict(lm.result,data.frame(conc = newconc), level = 0.9, interval = "confidence")
```

```
   fit       lwr        upr
 1 13.3  10.85809   15.74191
 2 32.7  30.92325   34.47675
 3 52.1  50.32325   53.87675
 4 71.5  69.05809   73.94191
 5 90.9  87.49778   94.30222
```

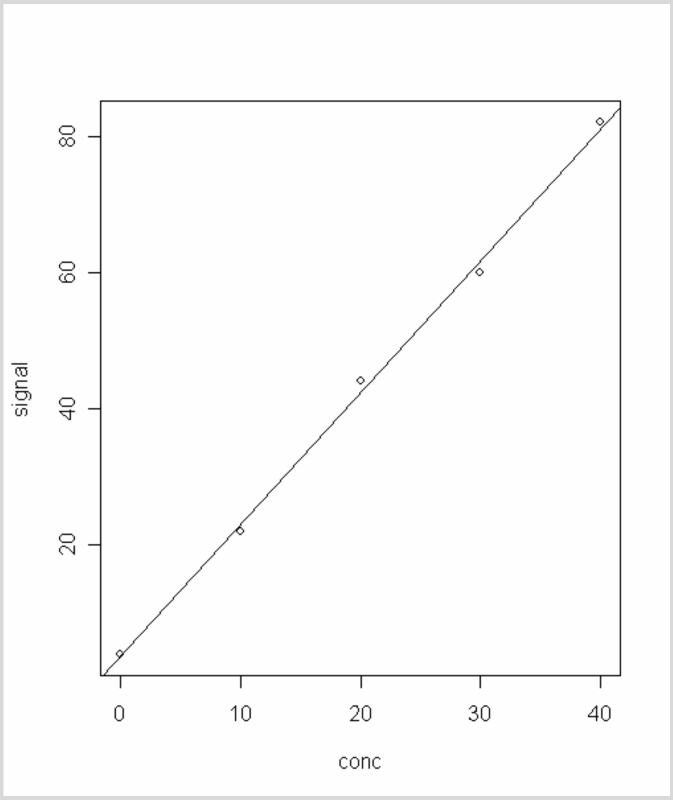
where ‘lwr’ is the lower limit of the confidence interval and ‘upr’ is the upper limit of the confidence interval. R does not contain a feature for finding the confidence intervals for predicted values of the independent variable for specified values of dependent variables, a common desire in chemistry. Too bad.

Adding Regression Lines to Plots

For straight-lines this is easy to accomplish.

```
> plot(conc, signal)
> abline(lm.r)
```

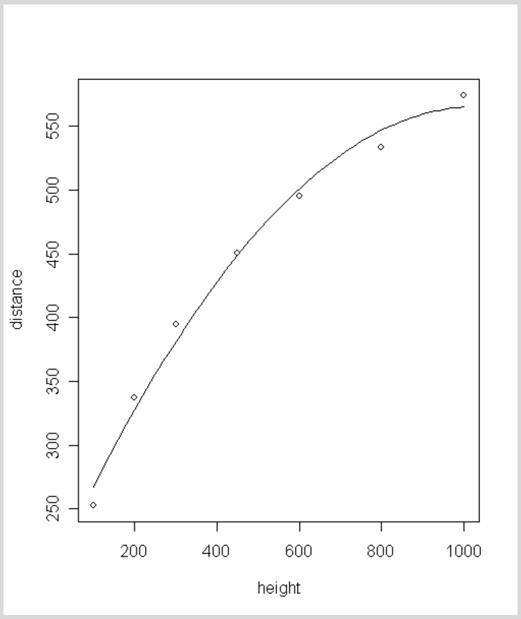
gives the following plot.



For data that does not follow a straight-line we must be more creative.

```
> height = c(100, 200, 300, 450, 600, 800, 1000)
> distance = c(253, 337, 395, 451, 495, 534, 574)                # data from Galileo

> lm.r = lm(distance ~ height + I(height^2)); lm.r               # a quadratic model

Call:
lm(formula = distance ~ height + I(height^2))

Coefficients:
(Intercept)        height    I(height^2)
 200.211950     0.706182    -0.000341

> newh = seq(100, 1000, 10); newh                                # create heights for
                                                                 # predictions

 [1]  100  110  120  130  140  150  160  170  180  190  200
[12]  210  220  230  240  250  260  270  280  290  300  310
[23]  320  330  340  350  360  370  380  390  400  410  420
[34]  430  440  450  460  470  480  490  500  510  520  530
[45]  540  550  560  570  580  590  600  610  620  630  640
[56]  650  660  670  680  690  700  710  720  730  740  750
[67]  760  770  780  790  800  810  820  830  840  850  860
[78]  870  880  890  900  910  920  930  940  950  960  970
[89]  980  990 1000

> fit = 200.211950 + 0.706182*newh - 0.000341*newh^2;fit         # calculate distance
                                                                 # for new heights
                                                                 # using model

 [1] 267.4201 273.7659 280.0434 286.2527 292.3938 298.4667 304.4715 310.4080
 [9] 316.2763 322.0764 327.8084 333.4721 339.0676 344.5949 350.0540 355.4450
[17] 360.7677 366.0222 371.2085 376.3266 381.3766 386.3583 391.2718 396.1171
[25] 400.8942 405.6032 410.2439 414.8164 419.3207 423.7568 428.1248 432.4245
[33] 436.6560 440.8193 444.9144 448.9414 452.9001 456.7906 460.6129 464.3670
[41] 468.0530 471.6707 475.2202 478.7015 482.1146 485.4595 488.7363 491.9448
[49] 495.0851 498.1572 501.1612 504.0969 506.9644 509.7637 512.4948 515.1578
[57] 517.7525 520.2790 522.7373 525.1274 527.4493 529.7031 531.8886 534.0059
[65] 536.0550 538.0359 539.9487 541.7932 543.5695 545.2776 546.9176 548.4893
[73] 549.9928 551.4281 552.7952 554.0941 555.3249 556.4874 557.5817 558.6078
[81] 559.5657 560.4555 561.2770 562.0303 562.7154 563.3323 563.8811 564.3616
[89] 564.7739 565.1180 565.3940

> plot(height, distance)                                         # original data
> lines(newh, fit, lty=1)                                        # display best fit
```

The resulting plot is shown here.


distance
height