A First Course on Kinetics and Reaction Engineering

Example S3.2

Problem Purpose

This example shows how to use the MATLAB script file FitLinmbSR.m to fit a linear model to experimental data.

Problem Statement

Assume that in the course of solving a kinetics problem, you have reached the point where you have data from eleven experiments, and that the data have been worked up to give the eleven data points listed in Table 1. The table shows that there is one set variable, x, and one response variable, $\hat{y}$. Suppose that you now need to determine whether equation (1) offers an accurate model for the data, and if it does, to determine the best values of m and b along with their uncertainties.

Table 1

x	$\hat{y}$
0	9.88
1	12.67
2	15.09
3	18.1
4	21.2
5	24.2
6	27.8
7	30.2
8	33.9
9	36.6
10	39.1

$$y = mx + b \qquad (1)$$

Problem Analysis

The model equation is linear with a single set variable and with a non-zero intercept. Therefore, the MATLAB script file FitLinmbSR.m can be used to fit the model to the experimental data.

Problem Solution

The first step is to import or enter the experimental data. The set variables must be stored in a column vector named x and the response variables in a column vector named y_hat. There should be one row per data point in these column vectors, as can be seen in Listings 1 and 2. At this point, provided that FitLinmbSR.m is located in the MATLAB search path, you simply need to type "FitLinmbSR" at the MATLAB command prompt to execute the script and perform the regression analysis. Doing so will generate the text output shown in Listing 3. It will also generate the model plot shown in Figure 1. The model equation is plotted as a red line, and the experimental data are plotted on the same axes as points. Because there are only two variables, total, in the model, there isn't any need to generate a parity plot or a plot of the residuals as a function of the set variable. Any information that could be gleaned from those plots can be found in the model plot that is generated.

```
>> FitLinmbSR

r_squared =
   0.9989


m =
   2.9914


m_u =
   0.0764


b =
   9.4741

b_u =
   0.4523
```

x =	y_hat =
0	9.8800
1	12.6700
2	15.0900
3	18.1000
4	21.2000
5	24.2000
6	27.8000
7	30.2000
8	33.9000
9	36.6000
10	39.1000

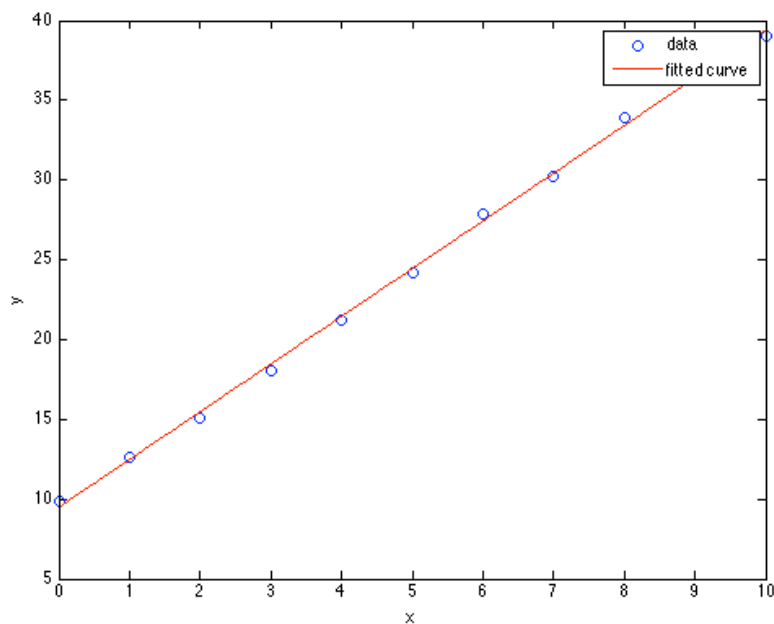*Listing 1.*   *Listing 2.*

Listing 3.

Figure 1. Plot of the fitted linear model and the data in Table 1.

From this output, you can see that the correlation coefficient, r^2, is equal to 0.9989 and the parameters have the following values and 95% confidence limits: m = 2.99 ± 0.08 and b = 9.47 ± 0.45. The correlation coefficient is very nearly equal to 1.0, so the fit appears to be very good, but we still should examine the model plot, Figure 1. As expected given the good correlation coefficient, the model plot shows all of the data points to be very close to the model line. In addition, there does not appear to be any systematic deviation of the data points from the line. Therefore, the fit can be deemed to be acceptable with the slope and intercept reported above.