

# A First Course on Kinetics and Reaction Engineering

## Example S3.3

### Problem Purpose

This example shows how to use the MATLAB script file FitLinmSR.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	-0.74
1	4.31
2	9.76
3	14.14
4	19.31
5	24.6
6	29.8
7	34.2
8	39.6
9	44.1
10	49.6

$$y = mx$$

(1)

### Problem Analysis

The model equation is linear with a single set variable and no intercept. Therefore, the MATLAB script file FitLinmSR.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  $y_{\text{hat}}$ . Column vector  $x$  must contain the values of the set variables, one per row and column vector  $y_{\text{hat}}$  must contain the values of the measured response variables, one per row, as shown in Listings 1 and 2. At this point, provided that `FitLinmSR.m` is located in the MATLAB search path, you simply need to type “FitLinmSR” 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. From the output you can see that the correlation coefficient,  $r^2$ , is equal to 0.9993 and the value of the slope is  $m = 4.92 \pm 0.05$ . The correlation coefficient is very nearly equal to 1.0, so the fit appears to be very good.

$x =$	$y_{\text{hat}} =$
0	-0.7400
1	4.3100
2	9.7600
3	14.1400
4	19.3100
5	24.6000
6	29.8000
7	34.2000
8	39.6000
9	44.1000
10	49.6000

Listing 1.

Listing 2.

```
>> FitLinmSR
r_squared =
    0.9993
m =
    4.9205
m_u =
    0.0486
```

Listing 3.

The script also generates a model plot with the set variable as the  $x$  axis and the response variable as the  $y$  axis. The model equation is plotted on these axes as a red line, and the experimental data are plotted on the same axes as points. Because there are only two variables 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. The plot that is generated for the data of this example is shown in Figure 1. As expected given the good correlation coefficient, the model plot shows all of the data points to be very close to the line for the model. In addition, the deviations of the data points from the line appear to be random, without any systematic trends. Therefore, the fit can be deemed to be acceptable with the slope reported above.

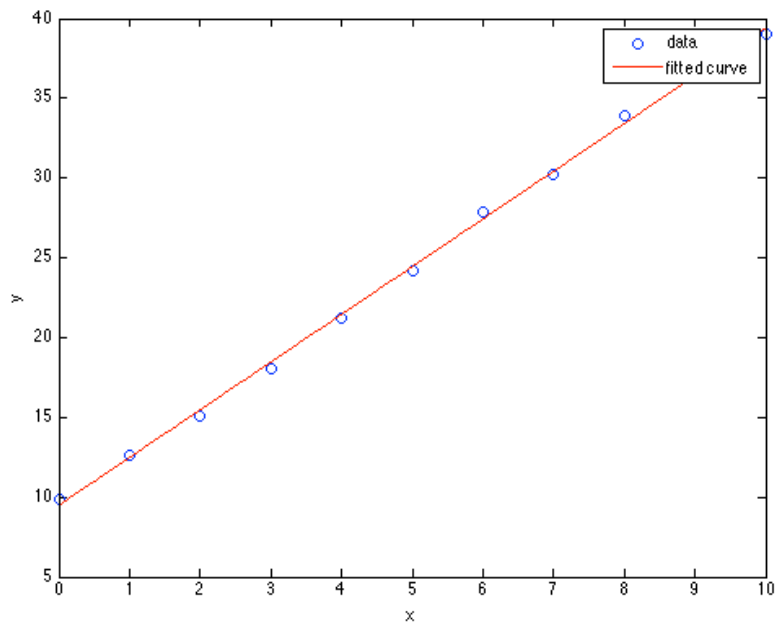


Figure 1. Plot of the fitted linear model and the data in Table 1.