Nonlinear Regression II

Physics 258 - DS Hamilton 2004

This example worksheet uses a generalized least-squares fitting procedure that is built into Mathcad to find the optimal fit parameters for an arbitrary (nonlinear) model function.

The data is from Taylor 2nd ed, problem 8.25. The rate at which a radioactive material emits radiation (and number of remaining radioactive nuclei) is expected to decrease exponentially with time. The two data vectors are "x", the elapsed time t (in min), and "y": the number of counts in a 15-second interval.

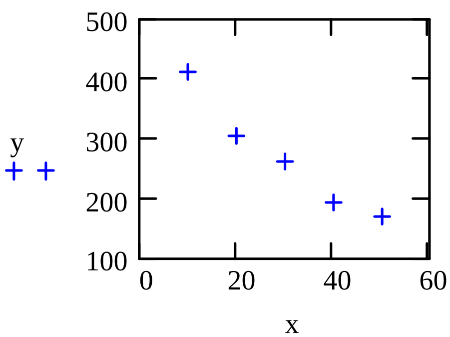
Raw Data:

$$x := \begin{pmatrix} 10 \\ 20 \\ 30 \\ 40 \\ 50 \end{pmatrix} \qquad y := \begin{pmatrix} 409 \\ 304 \\ 260 \\ 192 \\ 170 \end{pmatrix}$$

$n := \text{rows}(x)$ number of data points

$n = 5$

$i := 0 .. n - 1$ we will want to use this range variable later



Always plot the data before attempting a fit.

$$f(x, \alpha, \beta) := \alpha \cdot e^{\beta \cdot x}$$

This is the fitting function. The coefficient β will be negative and $|-1/\beta| = \tau$ is the lifetime for the radioactive decay.

$$dfd\alpha(x, \alpha, \beta) := e^{\beta \cdot x}$$

$$dfd\beta(x, \alpha, \beta) := x \cdot \alpha \cdot e^{\beta \cdot x}$$

Next, write down the partial derivatives of the function f with respect to the two parameters of interest, α & β.

$$F(x, a) := \begin{pmatrix} f(x, a_0, a_1) \\ dfd\alpha(x, a_0, a_1) \\ dfd\beta(x, a_0, a_1) \end{pmatrix}$$

Formulate a vector function that will be the argument to the "genfit" function.

$$a := \begin{pmatrix} 500 \\ -0.5 \end{pmatrix}$$

Initial guess for the two parameters. This is one reason to plot the data first.

$$\begin{pmatrix} \alpha \\ \beta \end{pmatrix} := \mathrm{genfit}(x, y, a, F)$$

Call the function "genfit" to find the best-fit coefficients.

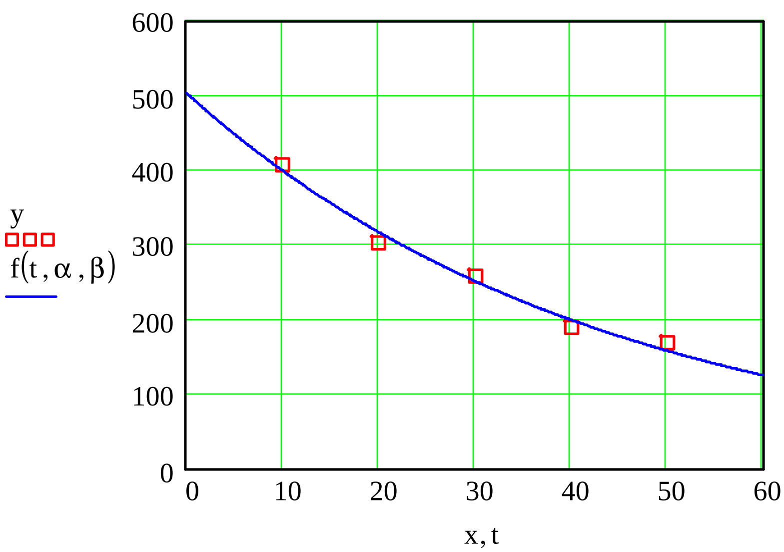
The solution is:

$\alpha = 505.3$ $\beta = -0.023$ $\frac{1}{\beta} = -43.392$

These are basically identical to those found in the "minssd" example.

$t := 0, 0.1 .. 60$

Use this dummy variable to plot the fit so that it looks like a smooth curve through 600 points.



$$SSD := \sum_i \left(y_i - f(x_i, \alpha, \beta)\right)^2$$

$$\sqrt{\frac{SSD}{n}} = 10.1$$

This is the RMS difference between the data pints and the fitting function.