Nonlinear Regression I

Physics 258 - DS Hamilton 2004

This example worksheet uses a generalized least-squares fit in 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.

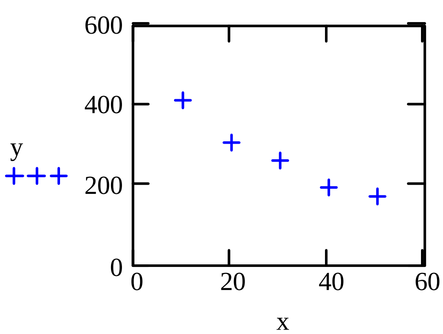
Raw Data:

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

$n := \text{rows}(x)$ 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.

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

The criteria for the "best fit" will be the one that minimizes the "Sum of Squared Differences". Use the range variable "i" to explicitly denote the x,y pairs.

$\alpha := 500 \qquad \beta := -0.5$

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

The solution for α and β should minimize the SSD. This minimization can be accomplished by using a "solve block". The solve block starts with the keyword "**Given**".

Given

$$SSD(\alpha,\beta) = 0$$

The "Minerr" function below finds the approximate solution to a system of (nonlinear) equations. We want find the approximate solution that is closest to the constraint SSD=0.

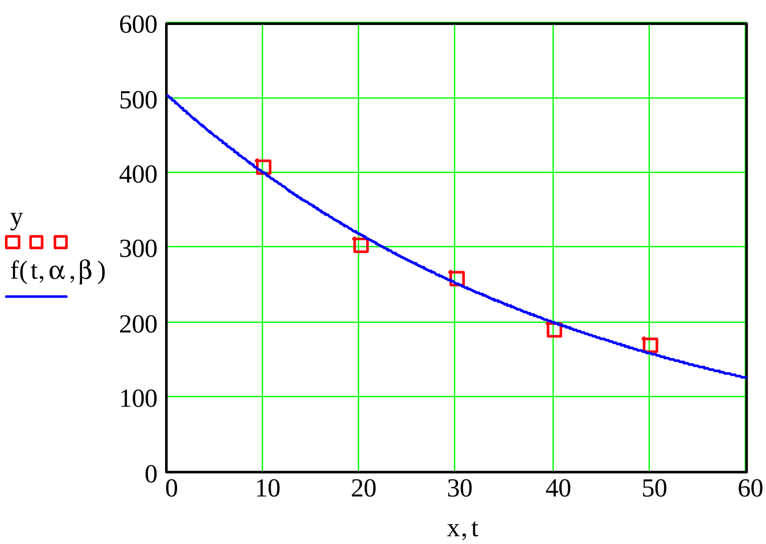
The solution is:

$$\begin{bmatrix} \alpha \\ \beta \end{bmatrix} := \text{Minerr}(\alpha,\beta)$$

$\alpha = 505.3$ $\beta = -0.023$ $\frac{1}{\beta} = -43.4$

$t := 0, 0.1 .. 60$

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



$$\sqrt{\frac{SSD(\alpha,\beta)}{n}} = 10.1$$

This is the RMS difference between the data points and the fitting function f(x,α,β).

$$\begin{bmatrix} a \\ b \end{bmatrix} := \text{Minimize}(SSD,\alpha,\beta) \qquad \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 505.3 \\ -0.023 \end{bmatrix}$$

The Minimize() function can also be used to minimize the SSD with respect to α and β, subject to no constraints.