



Nonlinear Regression III

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. I have included a weighting factor for each data point since they all do not have the same uncertainty σ_i .

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:

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

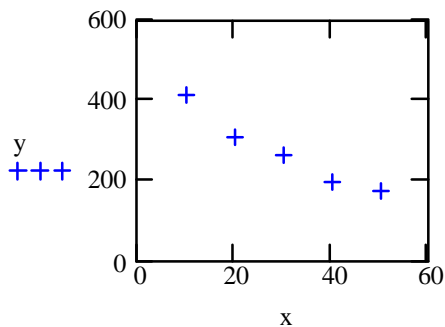
$n := \text{rows}(x)$

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.

$$\sigma_i := \sqrt{y_i}$$

For a counting experiment following Poisson statistics, the uncertainty is the square root of the number of counts.

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

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

$$\text{CHISQR}(\alpha, \beta) := \sum_i \left(\frac{y_i - f(x_i, \alpha, \beta)}{\sigma_i} \right)^2$$

The criteria for the "best fit" will be the one that minimizes the "Chi-squared". Use the range variable "i" to explicitly denote the x,y pairs.

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

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

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

Given

$$\text{CHISQR}(\alpha, \beta) = 0$$

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 CHISQR=0.

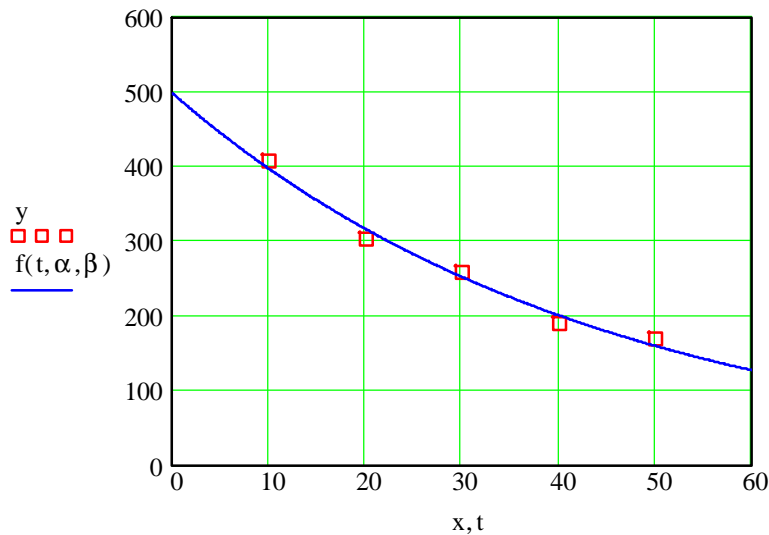
The solution is:

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

$$\alpha = 499.7 \quad \beta = -0.023 \quad \frac{1}{\beta} = -44.2$$

$$t := 0, 0.1 \dots 60$$

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



$$\text{CHISQR}(\alpha, \beta) = 2.051$$

$$\frac{\text{CHISQR}(\alpha, \beta)}{n - 2} = 0.684$$