Mee 390/490 : General Least-Square Curve Fitting

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Least square method (LSM) provides a procedure to calculate unknown coefficients (**c_j**) of a chosen function **f(x)** so that the sum of the square of "errors/deviations" (SSE), between fitted curve (an arbitrary chosen function) and given data (x,y) is minimal. The unknown coefficients may be determined numerically using MathCAD in at least three different ways (guessing the initial values of coefficients is necessary in all cases):

1. The SSE will be in extreme minimum if all partial derivatives of the SSE with respect to all coefficients are zeroes. That way the number of equations (partial derivatives equal zero) will always be equal t the number of unknown coefficients. Using the built-in "Given" and "Find" functions the coefficients may be calculated (if reasonably guessed, see NOTE 1 below). When cursor is on a function, pressing F1 key gives the "Help" on that function.

2. Using "Given" and "Minerr" function to solve for SSE=0 (even though it is not possible) will return the solution, i.e. the coefficients that will minimize the SSE.

3. Using the built-in "genfit" function for general curve-fitting of data (see FITTING ARBITRARY FUNCTIONS TO DATA in Help's Index Search.

The three methods will be illustrated on an example below:

Example: Find the best curve fit for the given data (x,y):

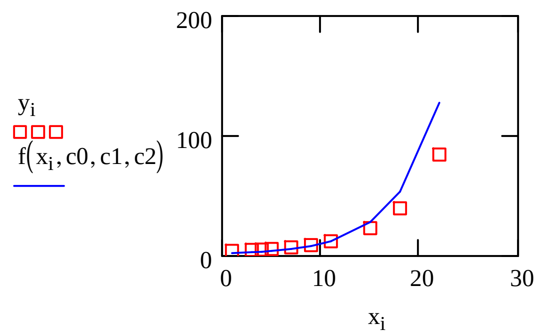
$$x := \begin{pmatrix} 1 \\ 3 \\ 4 \\ 5 \\ 7 \\ 9 \\ 11 \\ 15 \\ 18 \\ 22 \end{pmatrix} \quad y := \begin{pmatrix} 4.222 \\ 4.822 \\ 5.226 \\ 5.719 \\ 7.055 \\ 9.05 \\ 12.025 \\ 23.086 \\ 39.598 \\ 84.451 \end{pmatrix}$$

$$f(x, c0, c1, c2) := c0 + c1 \cdot \exp(c2 \cdot x)$$

...exponential function type, chosen arbitrarily on the bases of data plot shape.

The unknown coefficients are first guessed: $c0 := 1 \quad c1 := 1 \quad c2 := 0.22$

$$n := \text{length}(x) \quad n = 10 \quad i := 0..(n-1)$$



NOTE 1: If x-data are not in descending order, sorting functions must be use. Then data should be plotted, and type of function chosen to "match" the data "shape." Guess initial values for the coefficients (c_j) and plot the chosen function with guessed coefficients. Make adjustments (new guesses) if the match on the plot is unreasonable.

The SSE is:

$$SSE(c0, c1, c2) := \sum_i \left(f(x_i, c0, c1, c2) - y_i \right)^2$$

Partial derivative of SSE with regard to c0

$$DSE0(c0, c1, c2) := \sum_i \left[2 \cdot \left(f(x_i, c0, c1, c2) - y_i \right) \cdot (1) \right]$$

Partial derivative of SSE with regard to c1:

$$DSE1(c0, c1, c2) := \sum_i \left[2 \cdot \left(f(x_i, c0, c1, c2) - y_i \right) \cdot \left(\exp(c2 \cdot x_i) \right) \right]$$

Partial derivative of SSE with regard to c2:

$$DSE2(c0, c1, c2) := \sum_i \left[2 \cdot \left(f(x_i, c0, c1, c2) - y_i \right) \cdot \left(c1 \cdot x_i \cdot \exp(c2 \cdot x_i) \right) \right]$$

Method 1: Using "Given-Find" Functions

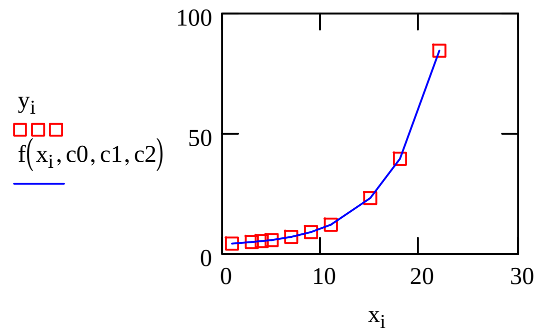
Given

$DSE0(c0, c1, c2) = 0$ ...partial derivative of SSE with regard to c0

$DSE1(c0, c1, c2) = 0$ ...partial derivative of SSE with regard to c1

$DSE2(c0, c1, c2) = 0$ ...partial derivative of SSE with regard to c2

$\begin{pmatrix} c0 \\ c1 \\ c2 \end{pmatrix} := \text{Find}(c0, c1, c2)$ $c0 = 3$ $c1 = 1$ $c2 = 0.2$



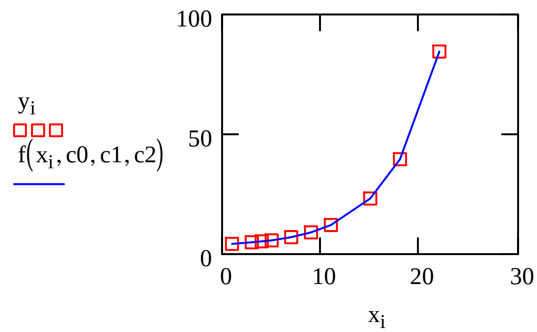
Method 2: Using "Given-Minerr" Functions

The coefficients are guessed: $c0 := 1$ $c1 := 1$ $c2 := 0.22$

Given

$SSE(c0, c1, c2) = 0$ $2 = 2$ $3 = 3$ NOTE 2: Additional dummy equations above are needed to match the number of coefficients.

$\begin{pmatrix} c0 \\ c1 \\ c2 \end{pmatrix} := \text{Minerr}(c0, c1, c2)$ $c0 = 3.004$ $c1 = 0.999$ $c2 = 0.2$



Method 3: Using "genfit" Functions

(see FITTING ARBITRARY FUNCTIONS TO DATA in Help's Index Search)

The coefficients are guessed $c0 := 1$ $c1 := 1$ $c2 := 0.22$

Coefficients' guesses:

$$cg := \begin{pmatrix} 1 \\ 1 \\ 0.22 \end{pmatrix} \qquad F(x, c) := \begin{pmatrix} c_0 + c_1 \cdot \exp(c_2 \cdot x) \\ 1 \\ \exp(c_2 \cdot x) \\ c_1 \cdot x \cdot \exp(c_2 \cdot x) \end{pmatrix}$$

...arbitrary curve-fit function $f(x,c_i)$

...partial derivative of $f(x,c_i)$ with regard to c_0

...partial derivative of $f(x,c_i)$ with regard to c_1

...partial derivative of $f(x,c_i)$ with regard to c_2

$$\begin{pmatrix} c0 \\ c1 \\ c2 \end{pmatrix} := \text{genfit}(x, y, cg, F) \qquad \begin{pmatrix} c0 \\ c1 \\ c2 \end{pmatrix} = \begin{pmatrix} 3 \\ 1 \\ 0.2 \end{pmatrix}$$