



Non-linear Regression - 2nd Order Polynomial Curve

The process of producing a mathematical function that provides the best fit to a series of experimental data points. The equation of the polynomial curve

A 2nd order polynomial quadratic regression:

$$y = a_0 + a_1 \cdot x + a_2 \cdot x^2$$

Experimental data

Raw data variables

(Independent variables)

(dependent variables)

$data :=$ <table style="border: 1px solid black; padding: 5px;"> <tr><td>-5</td><td>58.5</td></tr> <tr><td>-4</td><td>37.6</td></tr> <tr><td>-3</td><td>19.7</td></tr> <tr><td>-2</td><td>11.8</td></tr> <tr><td>-1</td><td>6.3</td></tr> <tr><td>0</td><td>3.6</td></tr> <tr><td>1</td><td>7.7</td></tr> <tr><td>2</td><td>13.6</td></tr> <tr><td>3</td><td>27.2</td></tr> <tr><td>4</td><td>40.9</td></tr> <tr><td>5</td><td>61.1</td></tr> </table>	-5	58.5	-4	37.6	-3	19.7	-2	11.8	-1	6.3	0	3.6	1	7.7	2	13.6	3	27.2	4	40.9	5	61.1	$x := col(data, 1) =$	$y_d := col(data, 2) =$
-5	58.5																							
-4	37.6																							
-3	19.7																							
-2	11.8																							
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3	27.2																							
4	40.9																							
5	61.1																							
	$\begin{bmatrix} -5 \\ -4 \\ -3 \\ -2 \\ -1 \\ 0 \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{bmatrix}$	$\begin{bmatrix} 58.5 \\ 37.6 \\ 19.7 \\ 11.8 \\ 6.3 \\ 3.6 \\ 7.7 \\ 13.6 \\ 27.2 \\ 40.9 \\ 61.1 \end{bmatrix}$																						

Total number of data points $n := length(x) = 11$

Summation of experimental data

Sum of x independent variables

$$sum_x := \sum_{i=1}^n x_i = 0$$

Sum of y dependent variables

$$sum_y := \sum_{i=1}^n y_{d_i} = 288$$

Sum of x raised to the power of 2 results

$$sum_{x^2} := \sum_{i=1}^n x_i^2 = 110$$

Sum of x raised to the power of 3 results

$$sum_{x^3} := \sum_{i=1}^n x_i^3 = 0$$

Sum of x raised to the power of 4 results

$$sum_{x^4} := \sum_{i=1}^n x_i^4 = 1958$$

Sum of x values multiplied by y values

$$sum_{xy} := \sum_{i=1}^n x_i \cdot y_{d_i} = 53.7$$

Sum of x squared values multiplied by y values

$$sum_{x^2y} := \sum_{i=1}^n x_i^2 \cdot y_{d_i} = 4783.7$$



Mean values for x and y variables

$$x_{mean} := \sum_{i=1}^n x_i \cdot n^{-1} = -5.5511 \cdot 10^{-17}$$

$$y_{mean} := \sum_{i=1}^n y_{d_i} \cdot n^{-1} = 26.1818$$

Matrices of least squares fitting - Sum of squares

$$M_1 := \begin{bmatrix} n & sum_x & sum_{xsq} \\ sum_x & sum_{xsq} & sum_{x3} \\ sum_{xsq} & sum_{x3} & sum_{x4} \end{bmatrix} = \begin{bmatrix} 11 & 0 & 110 \\ 0 & 110 & 0 \\ 110 & 0 & 1958 \end{bmatrix}$$

$$M_2 := \begin{bmatrix} sum_y \\ sum_{xy} \\ sum_{x2y} \end{bmatrix} = \begin{bmatrix} 288 \\ 53.7 \\ 4783.7 \end{bmatrix}$$

$$coeff := eval(M_1^{-1}) \cdot M_2 = \begin{bmatrix} 3.99417 \\ 0.48818 \\ 2.21876 \end{bmatrix}$$

Coefficients

$$\begin{cases} a_0 := coeff_1 \\ a_1 := coeff_2 \\ a_2 := coeff_3 \end{cases} = \begin{cases} 3.99417 \\ 0.48818 \\ 2.21876 \end{cases}$$

The residuals between the model and the data

$$res := y_d - a_0 - a_1 \cdot x - a_2 \cdot x^2 = \begin{bmatrix} -187.1174 \\ -208.5055 \\ -226.8937 \\ -235.2819 \\ -241.2701 \\ -244.4583 \\ -240.8465 \\ -235.4346 \\ -222.3228 \\ -209.111 \\ -189.3992 \end{bmatrix}$$

Check of results against the experimental data

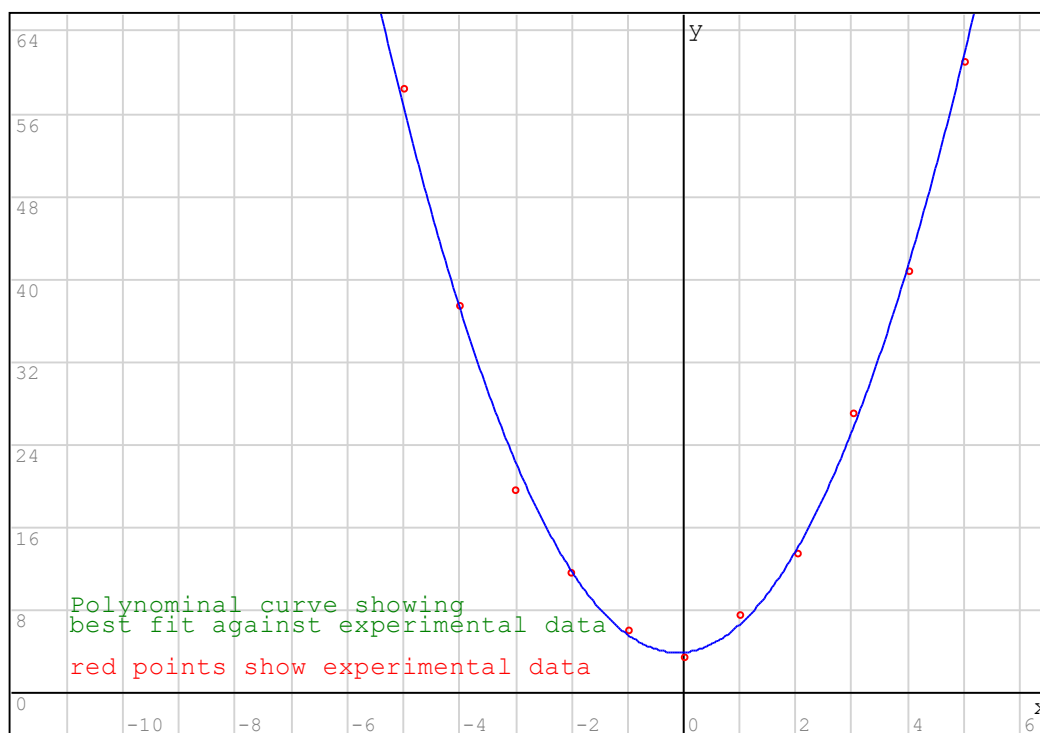
Calculated values

$$x = \begin{bmatrix} -5 \\ -4 \\ -3 \\ -2 \\ -1 \\ 0 \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{bmatrix} \quad y_d = \begin{bmatrix} 58.5 \\ 37.6 \\ 19.7 \\ 11.8 \\ 6.3 \\ 3.6 \\ 7.7 \\ 13.6 \\ 27.2 \\ 40.9 \\ 61.1 \end{bmatrix}$$

$$y := a_0 + a_1 \cdot x + a_2 \cdot x^2 + res = \begin{bmatrix} 58.5 \\ 37.6 \\ 19.7 \\ 11.8 \\ 6.3 \\ 3.6 \\ 7.7 \\ 13.6 \\ 27.2 \\ 40.9 \\ 61.1 \end{bmatrix}$$



$$f(x) := a_0 + a_1 \cdot x + a_2 \cdot x^2$$



Sum of squares of the residual

$$SS_{res} := \sum_{i=1}^n \left(y_{d_i} - a_0 - a_1 \cdot x_i - a_2 \cdot x_i^2 \right)^2$$

Total sum of the squares

$$SS_{tot} := \sum_{j=1}^n \left(y_j - y_{mean} \right)^2$$

R squared variance

$$R_{sq} := \frac{SS_{tot} - SS_{res}}{SS_{tot}} = 0.9963$$

Result for polynomial curve

$$y := a_0 + a_1 \cdot x + a_2 \cdot x^2$$

$$a_0 = 3.9942$$

$$a_1 = 0.4882$$

$$a_2 = 2.2188$$