



## Non-linear Regression - Exponential Curve

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

The equation of the exponential curve:  $y = A \cdot e^{b \cdot x}$

Experimental data

Raw data variables                      (Independent variables)                      (dependent variables)

$data :=$	<table style="border-collapse: collapse;"> <tr><td style="padding: 2px 10px;">1</td><td style="padding: 2px 10px;">0.0004</td></tr> <tr><td style="padding: 2px 10px;">2</td><td style="padding: 2px 10px;">0.001</td></tr> <tr><td style="padding: 2px 10px;">3</td><td style="padding: 2px 10px;">0.003</td></tr> <tr><td style="padding: 2px 10px;">4</td><td style="padding: 2px 10px;">0.007</td></tr> <tr><td style="padding: 2px 10px;">5</td><td style="padding: 2px 10px;">0.02</td></tr> <tr><td style="padding: 2px 10px;">6</td><td style="padding: 2px 10px;">0.054</td></tr> <tr><td style="padding: 2px 10px;">7</td><td style="padding: 2px 10px;">0.148</td></tr> <tr><td style="padding: 2px 10px;">8</td><td style="padding: 2px 10px;">0.403</td></tr> <tr><td style="padding: 2px 10px;">9</td><td style="padding: 2px 10px;">1.095</td></tr> <tr><td style="padding: 2px 10px;">10</td><td style="padding: 2px 10px;">2.978</td></tr> <tr><td style="padding: 2px 10px;">11</td><td style="padding: 2px 10px;">8.095</td></tr> </table>	1	0.0004	2	0.001	3	0.003	4	0.007	5	0.02	6	0.054	7	0.148	8	0.403	9	1.095	10	2.978	11	8.095	$x := \text{col}(data, 1) =$		$y_d := \text{col}(data, 2) =$		<table style="border-collapse: collapse;"> <tr><td style="padding: 2px 10px;">1</td><td style="padding: 2px 10px;">0.0004</td></tr> <tr><td style="padding: 2px 10px;">2</td><td style="padding: 2px 10px;">0.001</td></tr> <tr><td style="padding: 2px 10px;">3</td><td style="padding: 2px 10px;">0.003</td></tr> <tr><td style="padding: 2px 10px;">4</td><td style="padding: 2px 10px;">0.007</td></tr> <tr><td style="padding: 2px 10px;">5</td><td style="padding: 2px 10px;">0.02</td></tr> <tr><td style="padding: 2px 10px;">6</td><td style="padding: 2px 10px;">0.054</td></tr> <tr><td style="padding: 2px 10px;">7</td><td style="padding: 2px 10px;">0.148</td></tr> <tr><td style="padding: 2px 10px;">8</td><td style="padding: 2px 10px;">0.403</td></tr> <tr><td style="padding: 2px 10px;">9</td><td style="padding: 2px 10px;">1.095</td></tr> <tr><td style="padding: 2px 10px;">10</td><td style="padding: 2px 10px;">2.978</td></tr> <tr><td style="padding: 2px 10px;">11</td><td style="padding: 2px 10px;">8.095</td></tr> </table>	1	0.0004	2	0.001	3	0.003	4	0.007	5	0.02	6	0.054	7	0.148	8	0.403	9	1.095	10	2.978	11	8.095
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Total number of data points     $n := \text{length}(x) = 11$

finding the logs of the data will allow a linear relationship between x and y to be used

Mean values for x, y, log(x) and log(y)

$$x_{mean} := \sum_{i=1}^n x_i \cdot n^{-1} = 6$$

$$y_{mean} := \sum_{i=1}^n y_{d_i} \cdot n^{-1} = 1.1640$$

$$\ln x_{mean} := \sum_{i=1}^n \ln(x_i) \cdot n^{-1} = 1.5911$$

$$\ln y_{mean} := \sum_{i=1}^n \ln(y_{d_i}) \cdot n^{-1} = -2.8982$$

Least squares fitting - Sum of squares

$$SS_{\ln x} := \sum_{i=1}^n \ln(x_i) = 17.5023$$

$$SS_{\ln y} := \sum_{i=1}^n \ln(y_{d_i}) = -31.8797$$

$$SS_{\ln xy} := \sum_{i=1}^n x_i \cdot \ln(y_{d_i}) = -81.8984$$

$$SS_{x \ln sq} := \sum_{i=1}^n \ln(x_i)^2 = 33.4001$$

$$SS_x := \sum_{i=1}^n x_i = 66$$

$$SS_y := \sum_{i=1}^n y_{d_i} = 12.8044$$

$$SS_{x^2 y} := \sum_{i=1}^n x_i^2 \cdot y_{d_i} = 1401.6214$$

$$SS_{xy \ln y} := \sum_{i=1}^n x_i \cdot y_{d_i} \cdot \ln(y_{d_i}) = 213.1525$$



$$SS_{y \ln y} := \sum_{i=1}^n y_{d_i} \cdot \ln(y_{d_i}) = 19.3307$$

$$SS_{xy} := \sum_{i=1}^n x_i \cdot y_{d_i} = 133.4034$$

**Non-linear Regression (linearisation of a non-linear function)**

$$b := \frac{n \cdot SS_{\ln xy} - SS_{\ln x} \cdot SS_{\ln y}}{n \cdot SS_{x \ln sq} - SS_{\ln x}^2} = -5.6150$$

$$m := \ln y_{mean} - b \cdot \ln x_{mean} = 6.0360$$

Linearisation of  
Non-linear function

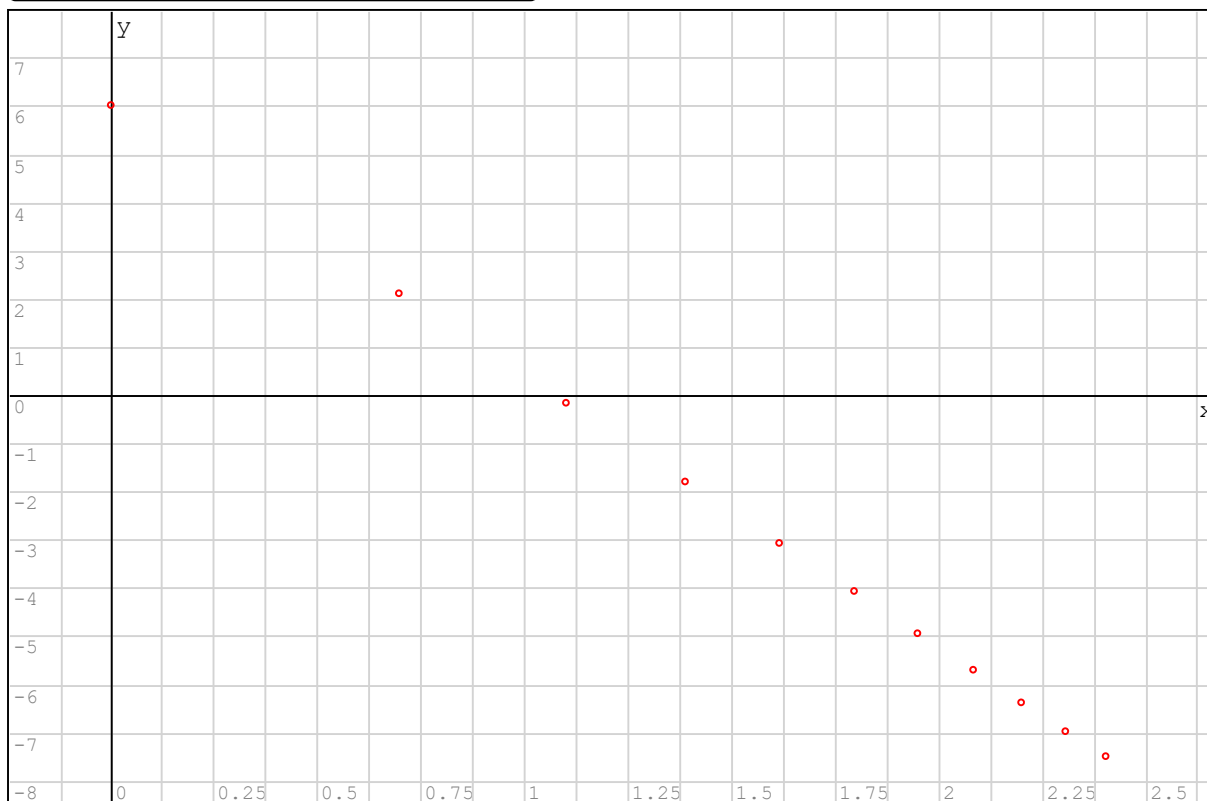
for  $i \in [1..n]$   
 $x_{\ln_i} := \ln(x_i)$

for  $i \in [1..n]$   
 $y_{\ln_i} := m + b \cdot \ln(x_i)$

$$x_{\ln} = \begin{bmatrix} 0 \\ 0.6931 \\ 1.0986 \\ 1.3863 \\ 1.6094 \\ 1.7918 \\ 1.9459 \\ 2.0794 \\ 2.1972 \\ 2.3026 \\ 2.3979 \end{bmatrix}$$

$$y_{\ln} = \begin{bmatrix} 6.036 \\ 2.144 \\ -0.1327 \\ -1.7481 \\ -3.001 \\ -4.0248 \\ -4.8903 \\ -5.6401 \\ -6.3015 \\ -6.8931 \\ -7.4282 \end{bmatrix}$$

Linearisation of non-linear function  
red points show experimental data





**Non-linear Regression (Exponential curve)**

$$y = A \cdot e^{b \cdot x}$$

$$a := \frac{SS_{x2y} \cdot SS_{ylny} - SS_{xy} \cdot SS_{xylny}}{SS_y \cdot SS_{x2y} - (SS_{xy})^2} = -8.9127$$

$$b := \frac{SS_y \cdot SS_{xylny} - SS_{xy} \cdot SS_{ylny}}{SS_y \cdot SS_{x2y} - (SS_{xy})^2} = 1.0004$$

$$A := e^{(a)} = 0.0001$$

Check of results against the experimental data

for  $i \in [1..n]$

$$y_i := A \cdot e^{b \cdot x_i}$$

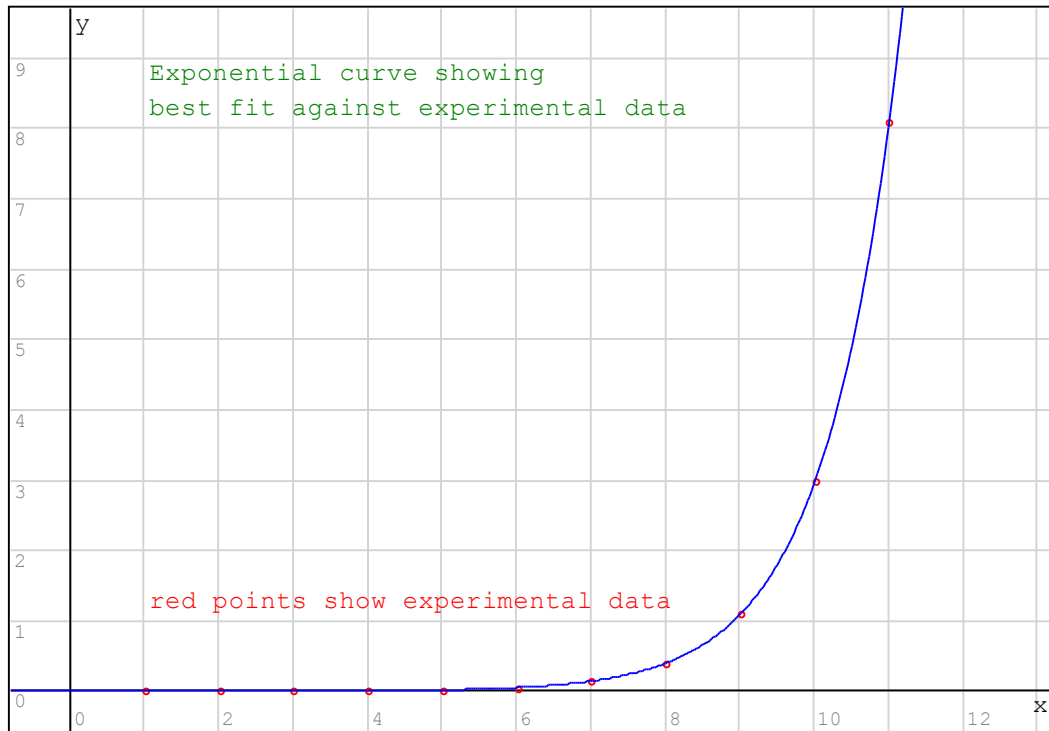
$$x = \begin{bmatrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ \vdots \end{bmatrix}$$

$$y_d = \begin{bmatrix} 0.0004 \\ 0.001 \\ 0.003 \\ 0.007 \\ 0.02 \\ 0.054 \\ 0.148 \\ 0.403 \\ \vdots \end{bmatrix}$$

Calculated values

$$y = \begin{bmatrix} 0.0004 \\ 0.001 \\ 0.0027 \\ 0.0074 \\ 0.02 \\ 0.0544 \\ 0.1481 \\ 0.4026 \\ \vdots \end{bmatrix}$$

$$f(x) := A \cdot e^{b \cdot x}$$



Sum of squares of the residual

$$SS_{res} := \sum_{i=1}^n \left( y_{d_i} - \left( A \cdot e^{b \cdot x_i} \right) \right)^2$$

Total sum of the squares

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

R squared variance

$$R_{sq} := \frac{SS_{tot} - SS_{res}}{SS_{tot}} = 1$$

**Result for exponential curve**

$$y := A \cdot e^{b \cdot x}$$

$$A = 0.0001$$

$$b = 1.0004$$