



## Non-Linear Regression - Saturation Growth Curve

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

The equation of the saturation growth rate curve:

$$y = a \cdot \frac{x}{b + x}$$

Experimental data

Raw data variables

(Independent variables)

(dependent variables)

data :=	5.0	16.0
	10.0	25.0
	15.0	32.0
	20.0	33.0
	25.0	38.0
	30.0	36.0
	35.0	39.0
	40.0	40.0
	45.0	42.0
	50.0	42.0

$$x := \text{col}(data, 1) = \begin{bmatrix} 5 \\ 10 \\ 15 \\ 20 \\ 25 \\ 30 \\ 35 \\ 40 \\ 45 \\ 50 \end{bmatrix}$$

$$y_d := \text{col}(data, 2) = \begin{bmatrix} 16.0 \\ 25.0 \\ 32.0 \\ 33.0 \\ 38.0 \\ 36.0 \\ 39.0 \\ 40.0 \\ 42.0 \\ 42.0 \end{bmatrix}$$

Total number of data points  $n := \text{length}(x) = 10$

Least squares fitting - Sum of squares

X = 1/x

$$X := \sum_{i=1}^n \frac{1}{x_i} = 0.5858$$

Y = 1/y

$$Y := \sum_{i=1}^n \frac{1}{y_{d_i}} = 0.3164$$

X squared

$$X_{sq} := \sum_{i=1}^n \left( \frac{1}{x_i} \right)^2 = 0.062$$

X \* Y

$$XY := \sum_{i=1}^n \frac{1}{x_i} \cdot \frac{1}{y_{d_i}} = 0.0244$$

Mean value of dependent variables

$$y_{mean} := n^{-1} \cdot \sum_{i=1}^n y_{d_i} = 34.3$$



**Non-linear Regression (Saturation Growth rate curve)**

$$y = a \cdot \frac{x}{b + x}$$

$$a_0 := \frac{n^{-1} \cdot Y \cdot X_{sq} - n^{-1} \cdot X \cdot XY}{X_{sq} - n^{-1} \cdot X^2} = 0.0191$$

$$a_1 := \frac{XY - n^{-1} \cdot X \cdot Y}{X_{sq} - n^{-1} \cdot X^2} = 0.2134$$

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

$$y_i := a \cdot \frac{x_i}{b + x_i}$$

$$a := \frac{1}{a_0} = 52.242$$

$$b := a_1 \cdot a = 11.1468$$

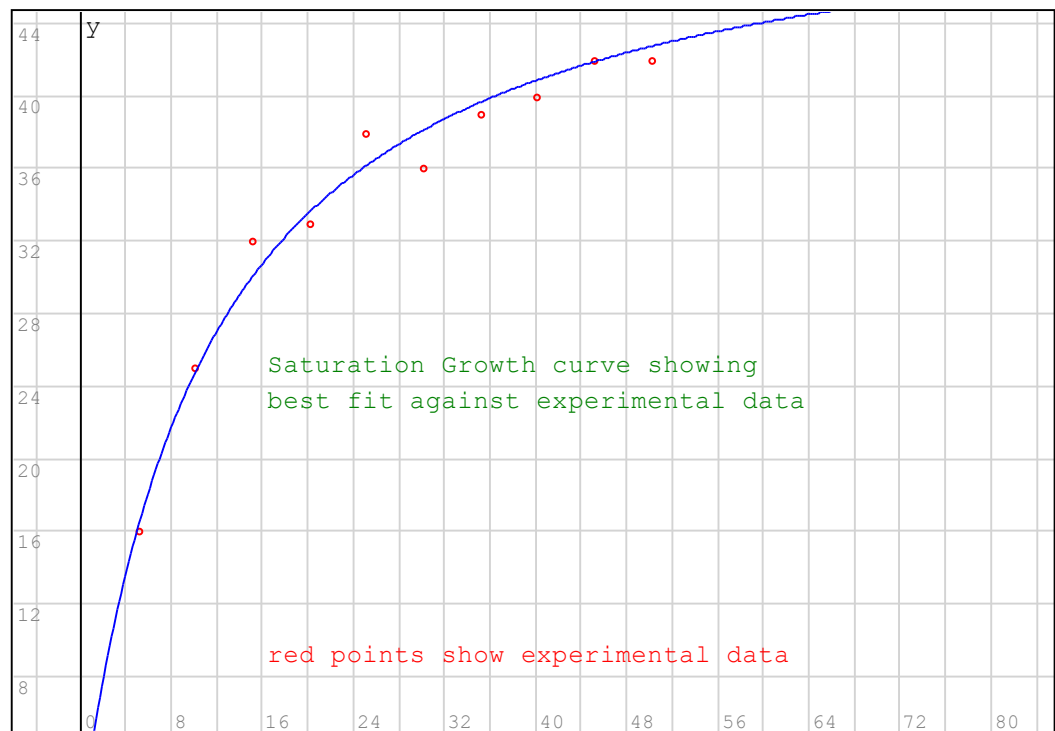
Check of results against the experimental data

Calculated values

Residuals

$x = \begin{bmatrix} 5 \\ 10 \\ 15 \\ 20 \\ 25 \\ 30 \\ 35 \\ \vdots \end{bmatrix}$	$y_d = \begin{bmatrix} 16 \\ 25 \\ 32 \\ 33 \\ 38 \\ 36 \\ 39 \\ \vdots \end{bmatrix}$	$y = \begin{bmatrix} 16.1772 \\ 24.7045 \\ 29.9704 \\ 33.5457 \\ 36.1318 \\ 38.0895 \\ 39.6229 \\ \vdots \end{bmatrix}$	$res := y_d - y = \begin{bmatrix} -0.1772 \\ 0.2955 \\ 2.0296 \\ -0.5457 \\ 1.8682 \\ -2.0895 \\ -0.6229 \\ \vdots \end{bmatrix}$
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$$f(x) := a \cdot \frac{x}{b + x}$$



Sum of squares of the residual

$$SS_{res} := \sum_{i=1}^n \left( y_d_i - a \cdot \frac{x_i}{b + x_i} \right)^2$$

Total sum of the squares

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

R squared variance

$$R_{sq} := \frac{SS_{tot} - SS_{res}}{SS_{tot}} = 0.9786$$

**Result for saturation growth curve**

$$y := a + b \cdot \ln(x)$$

$$a = 52.242$$

$$b = 11.1468$$