Version 10

FitAll

nonlinear regression analysis

Basic Functions Guide

MTR SOFTWARE

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Contents

Introduction

This ***FitAll***™ **Basic Functions Guide** describes the functions contained in the **.** Library and has an appendix that explains how to get help from ***MTR* Software**.

Function Reference Overview

This section describes each of the functions in ***FitAll***'s . Library.

In most cases, a graph of the function is shown. These graphs were created using "typical" parameter and constant values.

The actual appearance of a function depends on the parameter and constant values and may look quite different from the illustrations shown.

Equation

Gives the equation and its variations. The variations are listed in order of increasing complexity.

Constants

Lists the constants, K, that are used in the function. The default values for the constants also are given.

Parameters

Lists the parameters, P, that are used in the function.

Multi-Fits

Describes the Multi-Fit functionality of "Multi-Fit enabled" functions.

Sample Applications

Gives examples of some situations in which the function is known to be used.

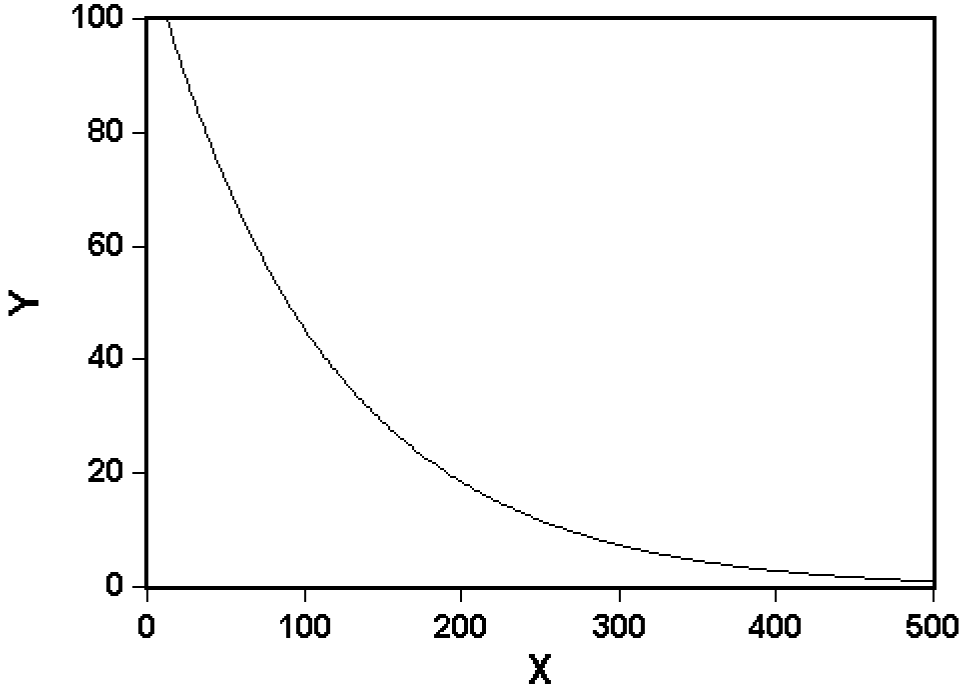
Remarks

Provides general comments and hints, and lists any known limitations or restrictions that should be observed when using the function.

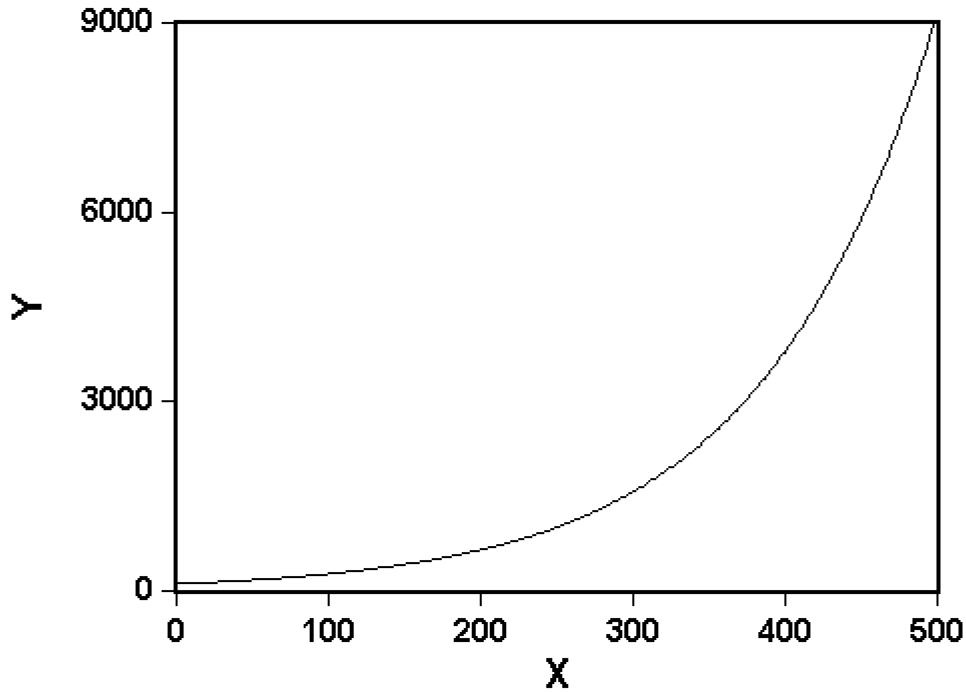
Also see

Provides links or references to other related functions.

Ftn 0001: First Order Exponential with Background Correction



or



Equation

$$Y = P1 * e^{(-P2 * K1 * X)} + \sum_{i=0}^{n} \left(P3 + i * X^{i}\right)$$

in which

- n can have values from 0 to 2.
- Y is the measured response.
- X is the independent variable, often the time.

For example:

- $Y = P1 * e^{-(P2 * K1 * X)}$
- $Y = P1 * e^{-(P2 * K1 * X)} + P3 + P4 * X$

Constants

Constant	Name	Comments
K1	K1	Default value is 1.0.

Parameters

Parameter	Name	Comments
P1	Yo-Yinf	Amplitude of the exponential. A positive value indicates that Y decreases as X increases in value.
P2	k	In kinetics k is the rate constant or 1/(time constant).
P3	Yinf	Value of Y when X is infinitely large.
P4	A1	Linear background correction term.
P5	A2	Quadratic background correction term.

Sample Applications

- Determining the rate constant of a chemical reaction.
- Determining the time constant (charging or discharging) of a RC circuit.
- May describe some simple diffusion processes.

Remarks

When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1, that is, the X-values.

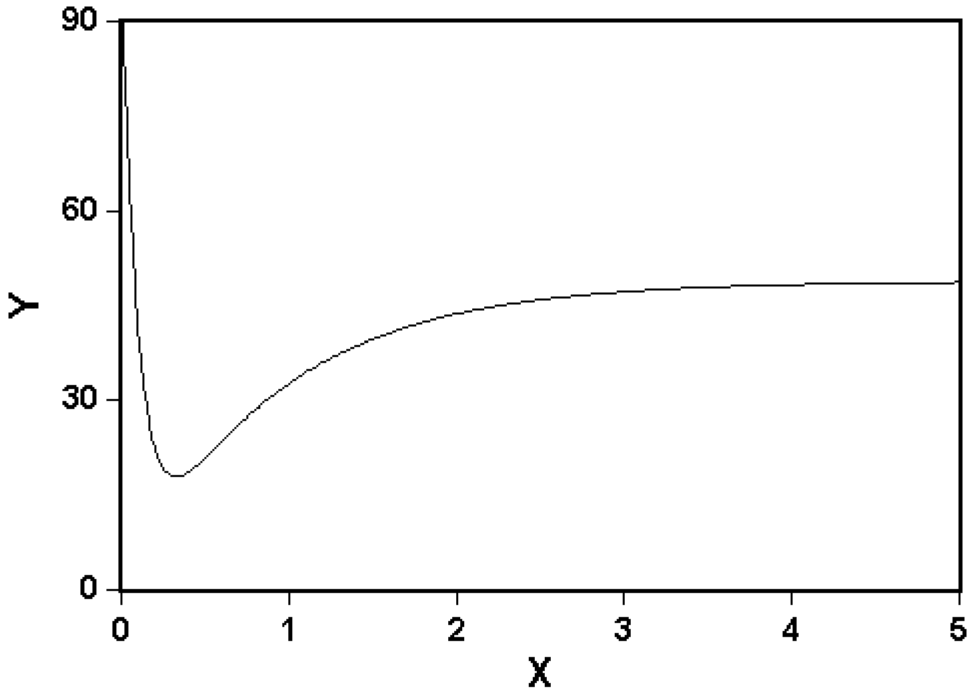
Also see

Function 0002 6

Function 0025 56

Function 0026 56

Ftn 0002: Sum of First Order Exponentials



Equation

The general form of the function is:

$$Y = P1 + \sum_{i=1}^{n} \left[P_{2i} * e^{-(P_{2i+1} * K_i * X)} \right]$$

in which

- n can have values from 1 to 5.
- Y is the measured response.
- X is the independent variable, often the time.

Five variations of the function are available. For example:

- $Y = P1 + P2 * e^{-(P3 * K1 * X)}$
- $Y = P1 + P2 * e^{-(P3 * K1 * X)} + P4 * e^{-(P5 * K2 * X)}$
- $Y = P1 + P2 * e^{-(P3 * K1 * X)} + P4 * e^{-(P5 * K2 * X)} + P6 * e^{-(P7 * K3 * X)}$

Constants

Constant	Name	Comments
K1	K1	Default value is 1.0.
K2	K2	Default value is 1.0.
K3	K3	Default value is 1.0.
K4	K4	Default value is 1.0.
K5	K5	Default value is 1.0.

Parameters

Parameter	Name	Comments
P1	Yinf	Value of Y when X is infinitely large.
P2	DeltaY1	Amplitude of the first exponential curve. Positive values indicate that Y decreases as X increases.
P3	k1	Rate constant, 1/(time constant), of the first exponential curve. Often has units of sec^{-1}.
P4	DeltaY2	Amplitude of the second exponential curve.
P5	k2	Rate constant, 1/(time constant), of the second exponential curve.
P6	DeltaY3	Amplitude of the third exponential curve.
P7	k3	Rate constant, 1/(time constant), of the third exponential curve.
P8	DeltaY4	Amplitude of the fourth exponential curve.
P9	k4	Rate constant, 1/(time constant), of the fourth exponential curve.
P10	DeltaY5	Amplitude of the fifth exponential curve.
P11	k5	Rate constant, 1/(time constant), of the fifth exponential curve.

Sample Applications

- Rates of two or more sequential, parallel, or overlapping reactions.

Remarks

Often the best fitting strategy is to fit the last (high X) part of the data using one exponential (equation a), then fit a larger segment of the data to two exponentials (equation b), and finally, if necessary, fit all of the data to three exponentials (equation c).

> **NOTE**:
> Ftn 0002a is the same as Ftn 0001b with the parameters arranged in a slightly different order.

Automatic initial estimates are available only when one exponential (Ftn 0002a) is selected.

When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1, that is, the X-values.

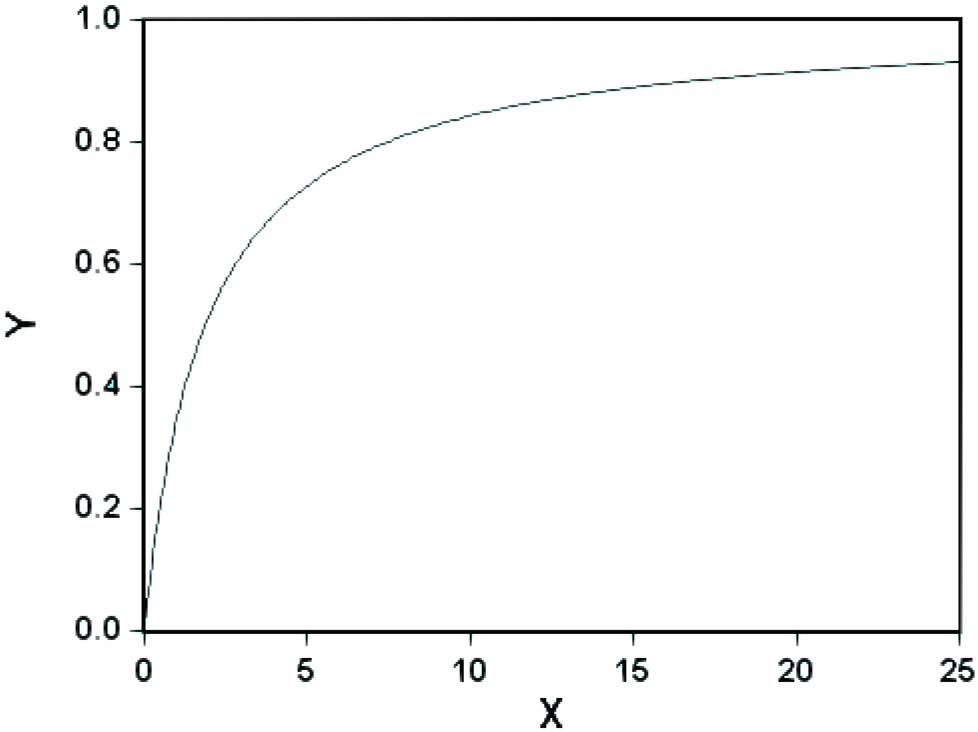
Also see

Function 0001 3

Function 0025 56

Function 0026 56

Ftn 0003: Langmuir Adsorption Isotherm



Equation

The function is:

$$Y = \frac{P1 * X}{(1 + P1 * X)}$$

in which:

- Y is the measured response.
- X is the independent variable.

Parameters

Parameter	Name	Comments
P1	K langmuir	Langmuir Adsorption Constant

Sample Applications

- Quantify the degree of adsorption of a corrosion inhibitor onto a surface.

Remarks

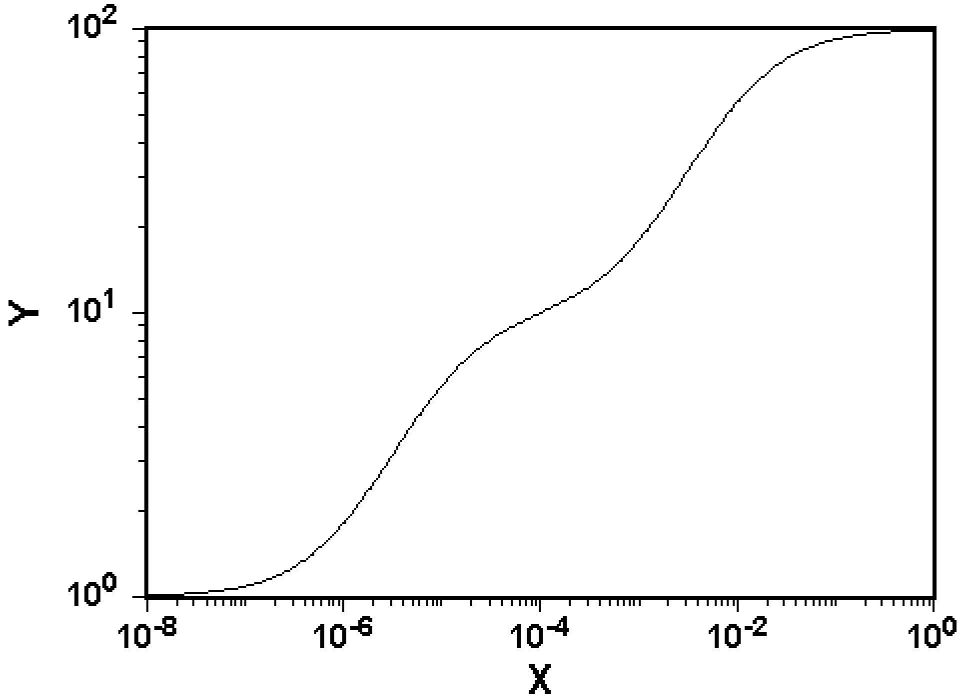
At fifty percent (50%) surface (site) coverage X = 1/P1.

At high values of X, the limiting value of Y is 1.0 .

At X = 0, Y = 0.

When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

Ftn 0004: Coupled Saturation Curves (Non Zero Origin)



Equation

The general form of the function is:

$$Y = \frac{P1 + \sum_{i=1}^{n}\left(X^{i} * P_{2i+1} * \prod_{j=1}^{i} P_{2j}\right)}{1 + \sum_{i=1}^{n}\left(X^{i} * \prod_{j=1}^{i} P_{2j}\right)}$$

in which:

- Y is the measured response.
- X is the independent variable.
- n can have values from 1 to 5.

Five variations of the function are available. For example:

- $$Y = \frac{(P1 + P2 * P3 * X)}{(1 + P2 * X)}$$

- $$Y = \frac{(P1 + P2 * P3 * X + P2 * P4 * P5 * X^2)}{(1 + P2 * X + P2 * P4 * X^2)}$$

- $$Y = \frac{(P1 + P2 * P3 * X + P2 * P4 * P5 * X^2 + P2 * P4 * P6 * P7 * X^3)}{(1 + P2 * X + P2 * P4 * X^2 + P2 * P4 * P6 * X^3)}$$

Parameters

Parameter	Name	Comments
P1	Yo	Limiting value of Y when X is zero.
P2	Q1	Equilibrium quotient (formation constant) for the first component.
P3	DeltaY1	Amplitude of Y for the first component. Positive values of DeltaY indicate that Y increases as the value of X increases. Negative values of DeltaY indicate that Y decreases as the value of X increases.
P4	Q2	Equilibrium quotient (formation constant) for the second component.
P5	DeltaY2	Amplitude of Y for the second component. Positive values of DeltaY indicate that Y increases as the value of X increases. Negative values of DeltaY indicate that Y decreases as the value of X increases.
P6	Q3	Equilibrium quotient (formation constant) for the third component.
P7	DeltaY3	Amplitude of Y for the third component.
P8	Q4	Equilibrium quotient (formation constant) for the fourth component.
P9	DeltaY4	Amplitude of Y for the fourth component.
P10	Q5	Equilibrium quotient (formation constant) for the fifth component.
P11	DeltaY5	Amplitude of Y for the fifth component.

Sample Applications

- Determining equilibrium (stability or formation) constants, Q_i, for the binding of a ligand or substrate to a metal ion, enzyme, or surface.
- Resolving equilibrium constants, Q_i, and rate constants, $DeltaY_i$, for a coupled reaction from the apparent rate constant's dependence on X.

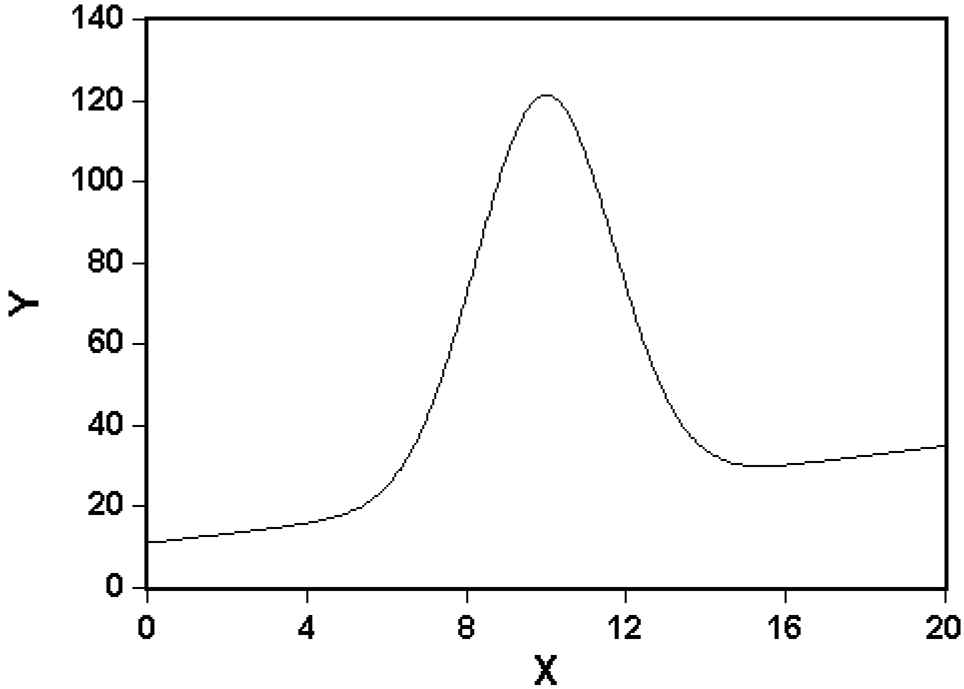
Remarks

Similar to Ftn 0003 9 except that the limiting values of Y at high and low X are not constrained to any particular values.

When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1, that is., the X-values.

FitAll will calculate initial estimates only when you are fitting the data to one saturation curve.

Ftn 0005: Gaussian With Background Correction



Equation

Four variations of the function are available:

- $Y = P1 * e^{\left[-2.77*\left(\frac{(X - P2)}{P3}\right)^2\right]}$
- $Y = P1 * e^{\left[-2.77*\left(\frac{(X - P2)}{P3}\right)^2\right]} + P4$
- $Y = P1 * e^{\left[-2.77*\left(\frac{(X - P2)}{P3}\right)^2\right]} + P4 + P5 * X$
- $Y = P1 * e^{\left[-2.77*\left(\frac{(X - P2)}{P3}\right)^2\right]} + P4 + P5 * X + P6 * X^2$

in which:

- Y is the measured response.

- X is the independent variable, often the concentration of a substance.

Parameters

Parameter	Name	Comments
P1	Ypeak	Maximum value of Y.
P2	Xpeak	Value of X when Y = Ypeak.
P3	FWHH	Full-Width at Half-Height. Width of the curve at Y = Ypeak/2.
P4	A0	Constant background offset.
P5	A1	Linear background correction term.
P6	A2	Quadratic background correction term.

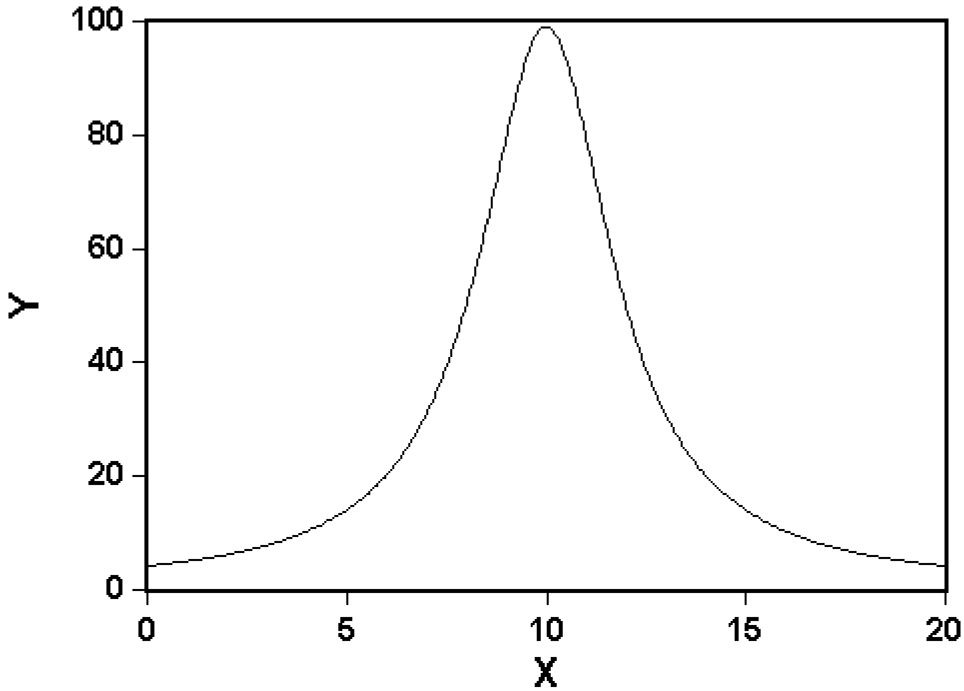
Sample Applications

- Fitting adsorption or emission peaks.
- Fitting chromatographic peaks.

Remarks

When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

Ftn 0006: Lorentzian With Background Correction



Equation

There are four variations of this function.

- $$Y = \frac{P1 * P3^2}{\left[4 * (X - P2)^2 + P3^2\right]}$$
- $$Y = \frac{P1 * P3^2}{\left[4 * (X - P2)^2 + P3^2\right]} + P4$$
- $$Y = \frac{P1 * P3^2}{\left[4 * (X - P2)^2 + P3^2\right]} + P4 + P5 * X$$
- $$Y = \frac{P1 * P3^2}{\left[4 * (X - P2)^2 + P3^2\right]} + P4 + P5 * X + P6 * X^2$$

in which:

- Y is the measured response.

- X is the independent variable, often the time or concentration of a substance.

Parameters

Parameter	Name	Comments
P1	Ypeak	Maximum value of Y.
P2	Xpeak	Maximum value of Y.
P3	FWHH	Full-Width at Half-Height. Width of the curve at Y = Ypeak/2.
P4	A0	Constant background offset.
P5	A1	Linear background correction term.
P6	A2	Quadratic background correction term.

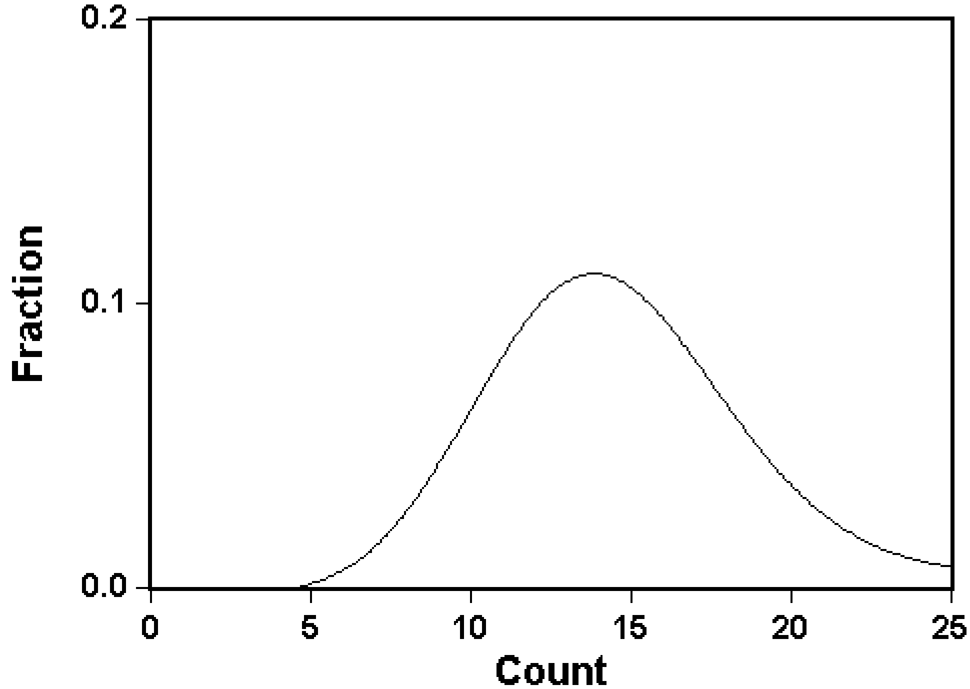
Sample Applications

- Fitting adsorption or emission peaks.

Remarks

When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

Ftn 0007: Poisson With Background Correction



Equation

There are four variations of the function:

- $Y = P2 * e^{[X * Ln(P1) - P1 - Ln(X!)]}$
- $Y = P2 * e^{[X * Ln(P1) - P1 - Ln(X!)]} + P3$
- $Y = P2 * e^{[X * Ln(P1) - P1 - Ln(X!)]} + P3 + P4 * X$
- $Y = P2 * e^{[X * Ln(P1) - P1 - Ln(X!)]} + P3 + P4 * X + P5 * X^2$

in which:

- Y is the measured response.
- X is the independent variable.

Parameters

Parameter	Name	Comments
P1	Xmean	Mean (average) value of the Poisson distribution.

Parameter	Name	Comments
		The standard deviation of a Poisson distribution is equal to the square root of the mean.
P2	NF	Normalization Factor: Amplitude scaling factor, such that Sum{Yi}/P2 = 1.0. If the Y-values correspond to the probability of observing X events per unit time, P2 should have a value of 1.
P3	A0	Constant background offset.
P4	A1	Linear background correction term.
P5	A2	Quadratic background correction term.

Remarks

All X-values must be greater than or equal to one (X >= 1).

When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1, that is, the X-values.

Ftn 0008: Multiple Linear: Y = Sum(Pj * Xij)

Equation

The general form of the function is:

$$Y_i = Po + \sum_j Pj * Xij$$

For example:

- Y = P0 + P1*X1 {a straight line)
- Y = P0 + P1*X1 + P2*X2
- Y = P1*X1 {a straight line with zero intercept}
- Y = P0 + P1*X1 + P2*X2 + P3*X3

in which:

- Y is the measured response.
- X is the independent variable.

Parameters

Parameter	Name	Comments
P1	P0	The number in the default name specifies the independent variable, Xi, that is multiplied by the parameter. P0 is a constant term.
P2	P1	This parameter is multiplied by the first independent variable, X1.
P3	P2	This parameter is multiplied by the second independent variable, X2.
P4	P3	This parameter is multiplied by the third independent variable, X3.
etc.	etc.	etc.

Sample Applications

- Correlating the relationship between the number and positions of substituents in a series of related chemicals with the rate (or log rate) of a chemical reaction.

- Correlating an overall market or economic trend with (proposed or possible) constituent market or economic indicators. That is, Y would be a measure of the overall market or economic value and each Xi (that is, X1, X2, etc.) would be the constituent indicators.

For example:

Y = Price of a stock

X1 = DOW Jones index.

X2 = Consumer Price Index.

X3 = Federal Reserve Discount Rate.

X4 = Business quarter (1, 2, 3, or 4th quarter).

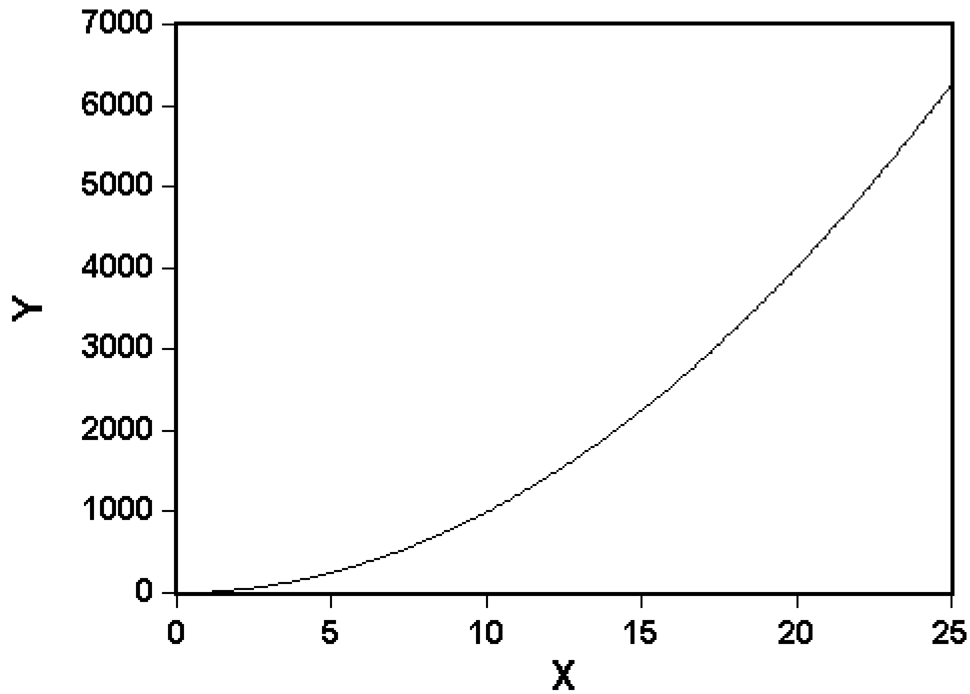
Remarks

Initial estimates are not required for this function because it is linear in its parameters.

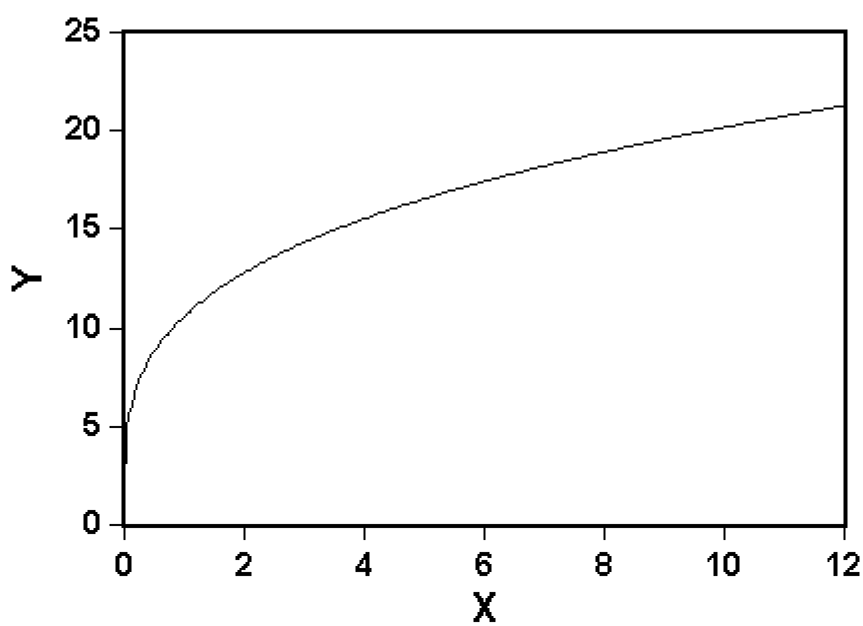
Also see

Function 0024: Multiple Linear_2 52

Ftn 0009: Power Curve: Y = P1 * X^P2 + P3



OR



Equation

Two variations of the function are available:

- $Y = P1 * X^{P2}$
- $Y = P1 * X^{P2} + P3$

in which:

- Y is the measured response.
- X is the independent variable.

Parameters

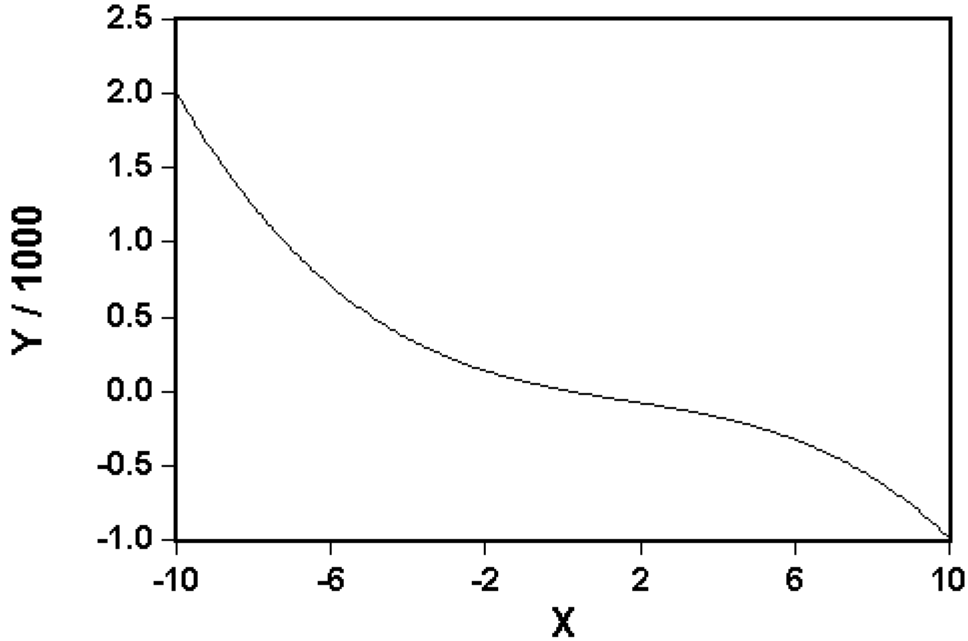
Parameter	Name	Comments
P1	A	Amplitude
P2	B	Exponent
P3	C	Intercept, value of Y at X = 0.

Remarks

The X-values must be positive; that is, X >= 0.

When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

Ftn 0010: Rational Function



Equation

The general form of the function, with at least one parameter in the numerator, is:

$$Y = \frac{PN0 + \sum_{i=1}^{n1} \left(PN_i * X^i\right)}{1 + \sum_{j=1}^{n2} \left(PD_j * X^j\right)}$$

in which:

- Y is the measured response.
- X is the independent variable.

For example:

- $Y = PN0 + PN1 * X$
- $Y = \frac{PN0}{(1 + PD1 * X)}$

Parameters

Parameter	Name	Comments
P1	PNi	Default name for parameters in the numerator. The value of i indicates the power of X.
P2	PDj	Default name for parameters in the denominator. The value of j indicates the power of X.

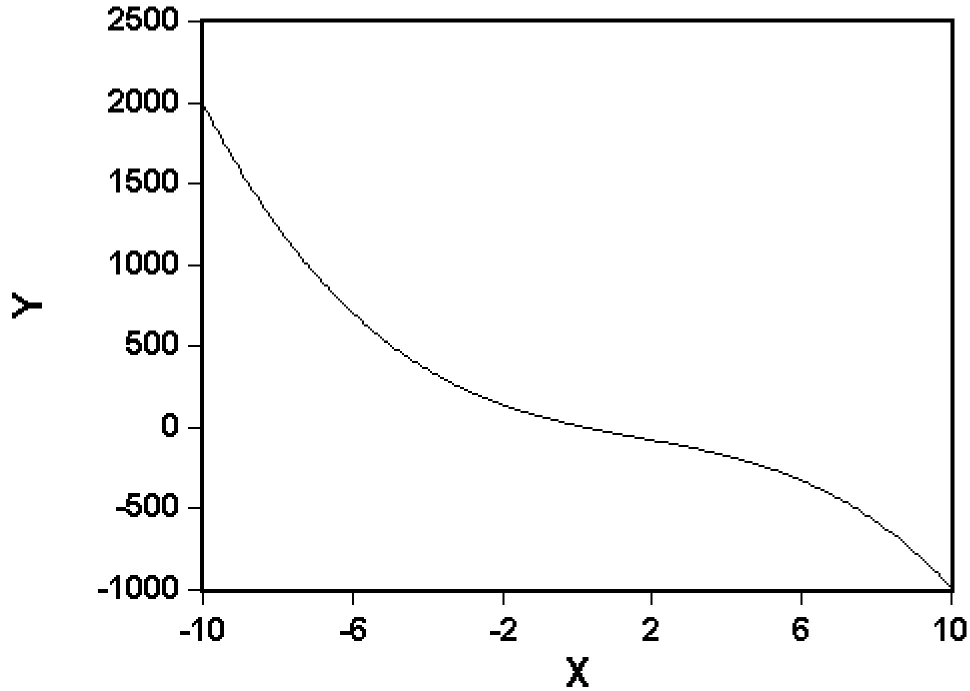
Sample Applications

- General purpose curve fits for the construction of calibration curves.

Remarks

Combinations of PNi and PDj parameters can be used up to a maximum of ten (10) parameters in total.

Ftn 0011: Polynomial_1



Equation

The general form of the function is:

$$Y = \sum_j P_j * X^j, \quad \text{for} -10 <= j <= 10$$

in which:

- Y is the measured response.
- X is the independent variable.

For example:

- $Y = P0 + P1 * X + P2 * X^2 + P3 * X^3$
- $Y = P0 + P1 * X \qquad \{\text{A straight line.}\}$
- $Y = P2 * X^2 + P3 * X^3 + P4 * X^4$
- $Y = \frac{P[-1]}{X} + P0 + P1 * X$

Parameters

Parameter	Name	Comments
	P_j	The "j" in the default names correspond to the power of X.

Sample Applications

- Empirical correlation for the construction of a calibration curve.

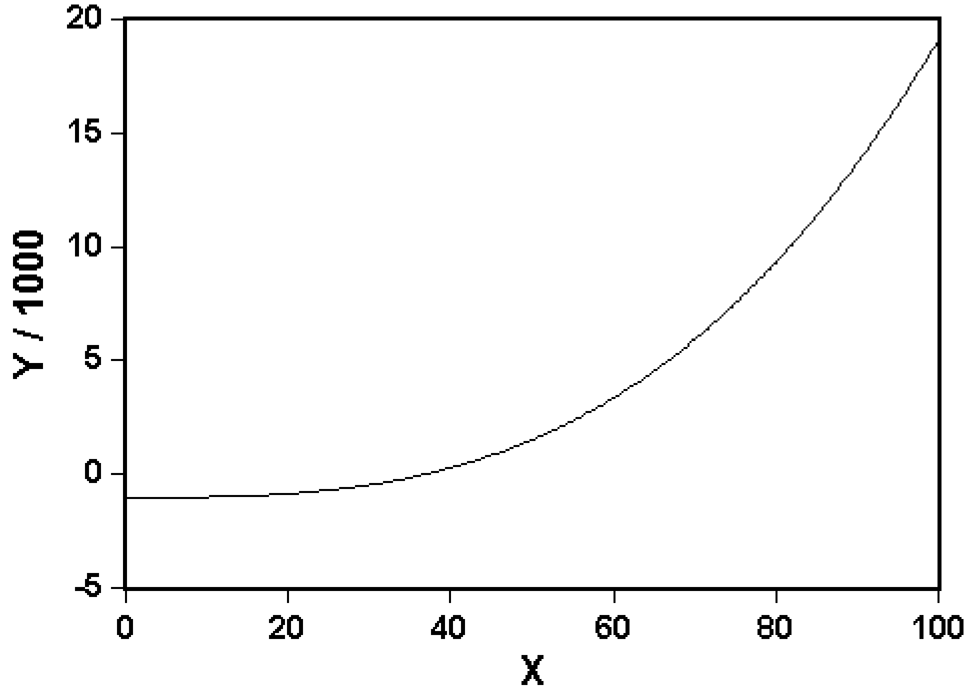
Remarks

It is generally best to use a polynomial with as few terms as possible.

Also see

Function 0012 28

Ftn 0012: Polynomial_2



Equation

The general form of the function is:

$$Y = \sum_{j=1}^{n} \left(P_j * |X|^{K_j} \right)$$

in which:

- Y is the measured response.
- X is the independent variable, often the time in seconds.

For example:

- $Y = P1 * |X|^{K1} + P2 * |X|^{K2} + P3 * |X|^{K3}$
- $Y = P1 * |X|^{K1} + P2 * |X|^{K2} + P3 * |X|^{K3} + P4 * |X|^{K4}$

Constants

Constant	Name	Comments
	K_j	The "j" in the default name indicates which parameter, P_j, is multiplied by X^K_j

Parameters

Parameter	Name	Comments
	P_j	The "j" in the default name indicates which constant, K_j, is used as the exponent of X.

Sample Applications

- Empirical correlation for the construction of a calibration curve.

Remarks

The exponent of X, K_j, does not have to be an integer. For example, K_j, can be assigned values such as 0.25, 0.5, 1 or -0.5.

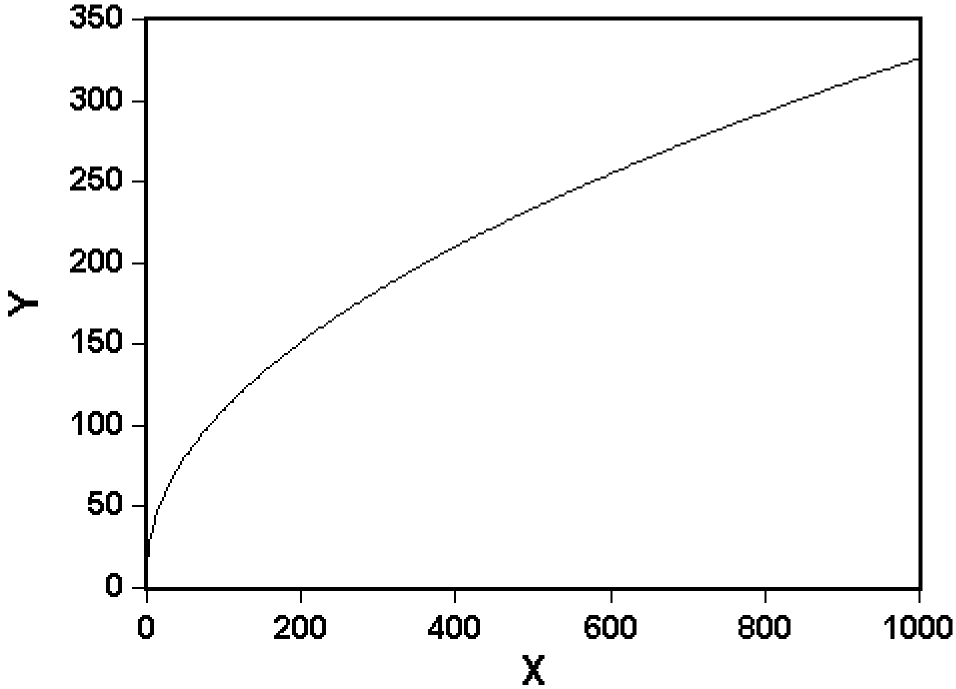
All values of X *must be greater than or equal to zero*, X >= 0.

It is generally best to use a polynomial with as few terms as possible.

Also see

Function 0011 26

Ftn 0013: Square Root: Y = P1 + P2 * |X|^1/2



Equation

$$Y = P1 + P2 * \sqrt{|X|}$$

in which:

- Y is the measured response.
- X is the independent variable, often the time in seconds.

Parameters

Parameter	**Name**	**Comments**
P1	P1	Intercept at X = 0.
P2	P2	Amplitude

Sample Applications

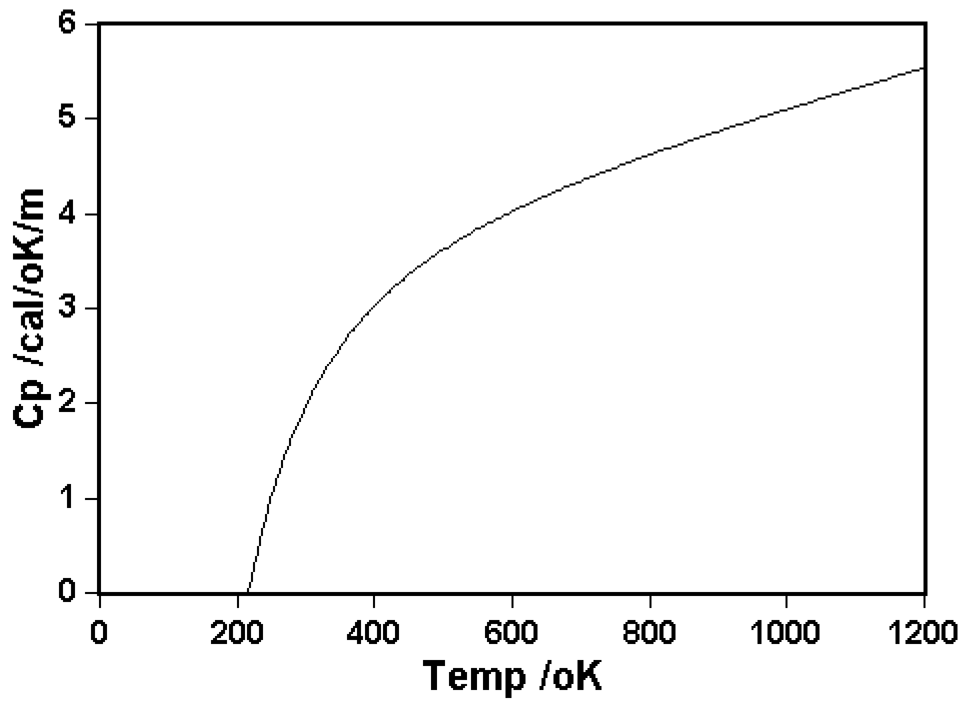
- The time dependence of some chemical reactions follow a square root (half-order) rate law (see function 0044).
- Some diffusion processes exhibit a square root time dependence.

Remarks

Only valid for X >= 0, if negative values of X are encountered, they are treated as positive values.

When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

Ftn 0014: Y = P1 + P2 * X + P3 / X^2



Equation

$$Y = P1 + P2 * \sqrt{|X|}$$

in which:

- Y is the measured response.
- X is the independent variable.

Parameters

Parameter	Name	Comments
P1	A	Intercept at X = 0.
P2	B	
P3	C	

Sample Applications

- Determining the temperature dependence of heat capacities, Cp.

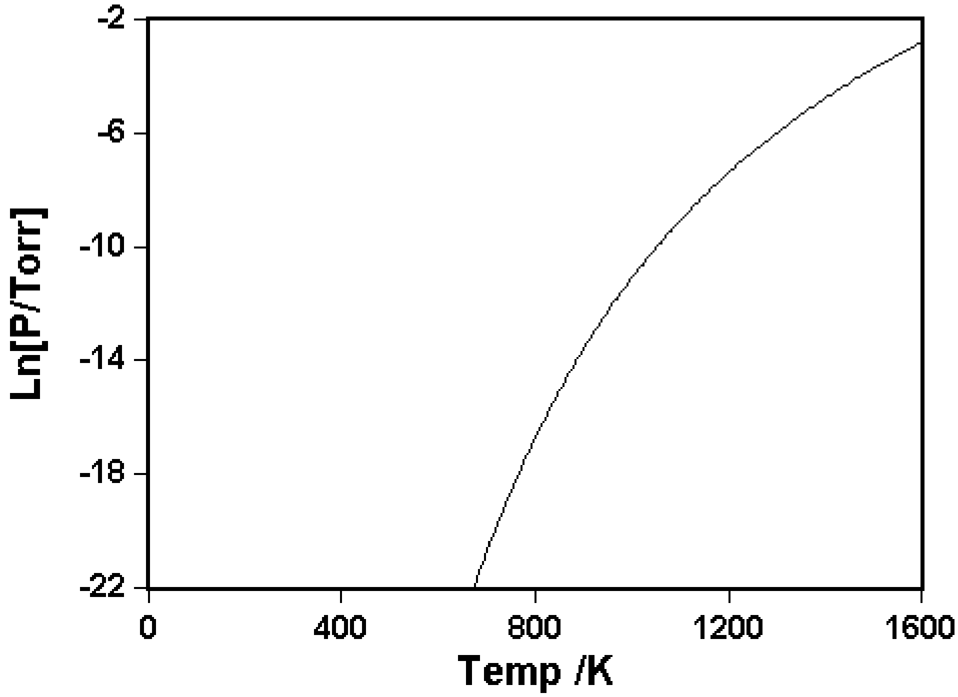
Remarks

The temperature, X, usually has units of degrees Kelvin, ^{o}K.

At X = 0, the function is not defined.

When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

Ftn 0015: Y = P1 + P2 / X + P3 * Ln|X|



Equation

$$Y = P1 + \frac{P2}{X} + P3 * Ln|X|$$

in which:

- Y is the measured response.
- X is the independent variable.

Parameters

Parameter	Name	Comments
P1	A	
P2	B	
P3	C	

Sample Applications

- Determining the temperature dependence of heat capacities, Cp.

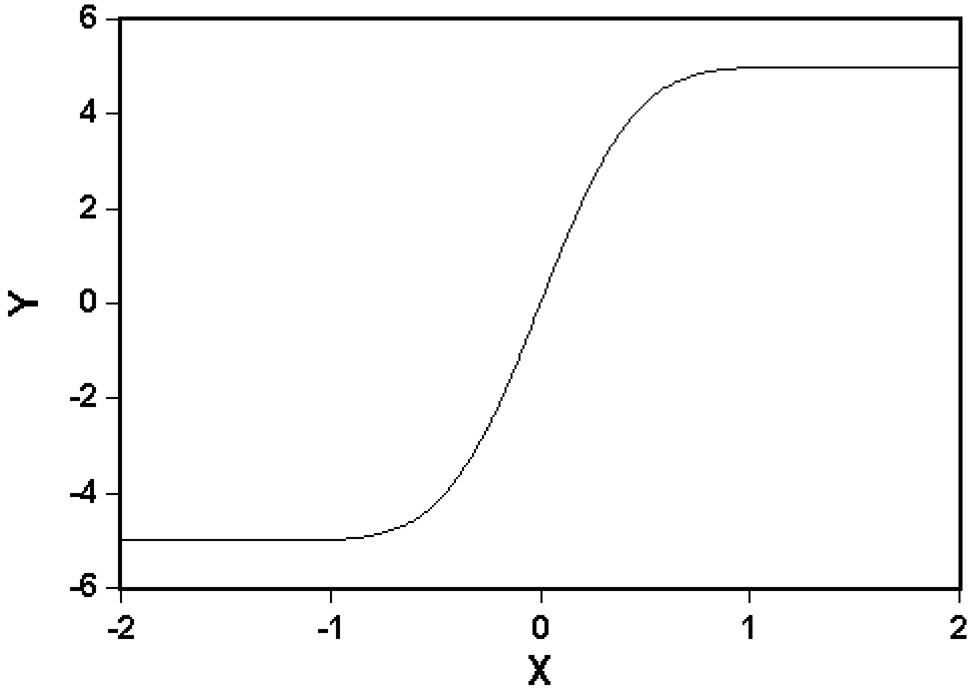
Remarks

The temperature, X, usually has units of degrees Kelvin, ^{o}K.

At X = 0, the function is **not** defined.

When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

Ftn 0016: Error Function (Erf) With Background Correction



Equation

The erf function is a special case of the incomplete gamma function, GammaP, and is defined as:

$$\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{(-t^2)}\, dt$$

There are four variations of this function:

- $Y = P1 * \mathrm{erf}(P2 * X)$
- $Y = P1 * \mathrm{erf}(P2 * X) + P3$
- $Y = P1 * \mathrm{erf}(P2 * X) + P3 + P4 * X$
- $Y = P1 * \mathrm{erf}(P2 * X) + P3 + P4 * X + P5 * X^2$

in which:

- Y is the measured response.
- X is the independent variable.

Parameters

Parameter	Name	Comments
P1	P1	Amplitude scaling factor.
P2	P2	
P3	A0	Constant background offset.
P4	A2	Linear background correction term.
P5	A3	Quadratic background correction term.

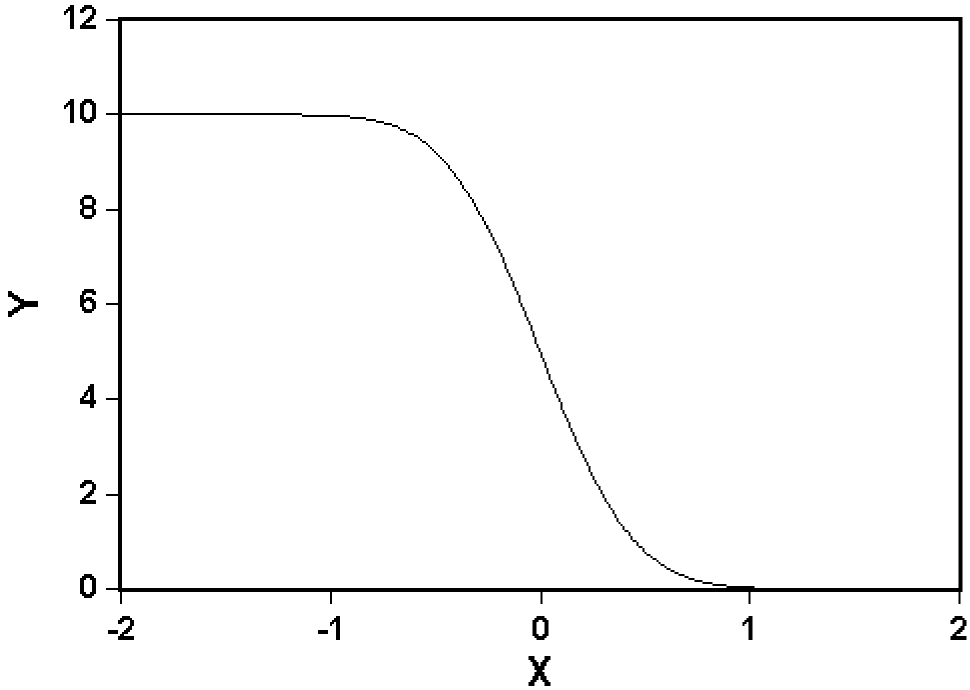
Sample Applications

- The erf and erfC functions can be used to describe some diffusion processes, for example, carburizing in metallurgy.

Remarks

When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

Ftn 0017: Complementary Error Function With Background Correction



Equation

The erfC function is a special case of the incomplete gamma function, GammaP, and is defined as:

$$\mathrm{erfC}(x) = 1 - \mathrm{erf}(x) = \frac{2}{\sqrt{\pi}} \int_x^{\infty} e^{\left(-t^2\right)}\, dt$$

There are four variations of this function:

- $Y = P1 * \mathrm{erfC}(P2 * X)$
- $Y = P1 * \mathrm{erfC}(P2 * X) + P3$
- $Y = P1 * \mathrm{erfC}(P2 * X) + P3 + P4 * X$
- $Y = P1 * \mathrm{erfC}(P2 * X) + P3 + P4 * X + P5 * X^2$

in which:

- Y is the measured response.
- X is the independent variable.

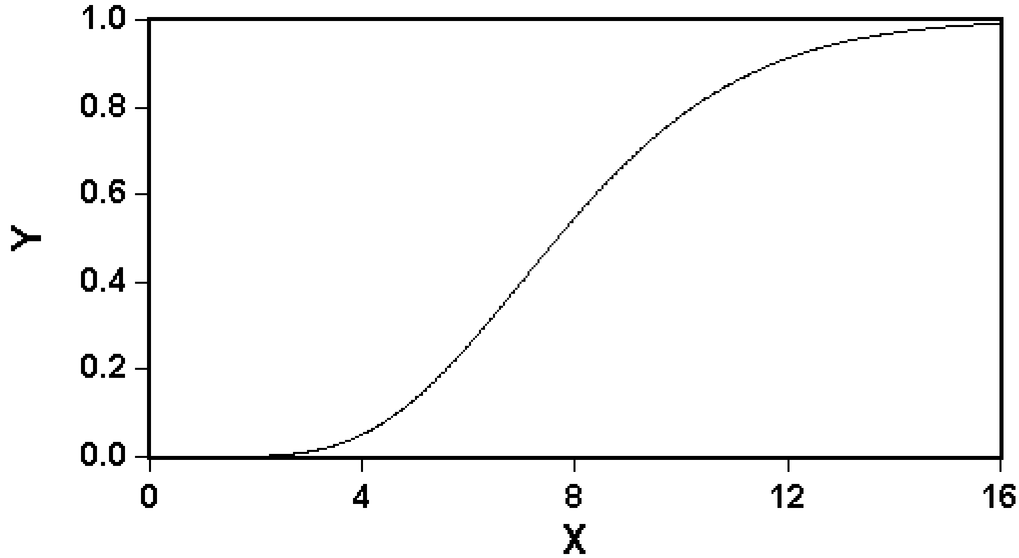
Parameters

Parameter	Name	Comments
P1	P1	Amplitude scaling factor.
P2	P2	
P3	A0	Constant background offset.
P4	A2	Linear background correction term.
P5	A3	Quadratic background correction term.

Remarks

When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

Ftn 0018: Incomplete Gamma Function (GammaP) With Background Correction



Equation

The incomplete gamma function, GammaP, is defined as:

$$\mathrm{GammaP}(a, x) = \frac{1}{\Gamma(a)} \int_0^x e^{-t} e^{a-1} \, dt$$

There are four variations of this function:

- $Y = P1 * \mathrm{GammaP}(P2, X)$
- $Y = P1 * \mathrm{GammaP}(P2, X) + P3$
- $Y = P1 * \mathrm{erfC}(P2 * X) + P3 + P4 * X$
- $Y = P1 * \mathrm{GammaP}(P2, X) + P3 + P4 * X + P5 * X^2$

in which:

- Y is the measured response.
- X is the independent variable.

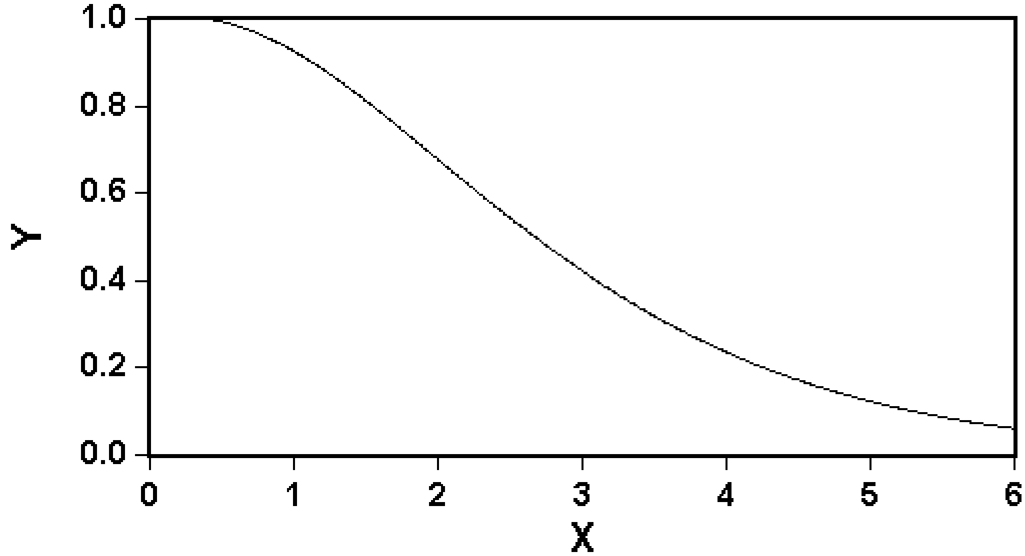
Parameters

Parameter	Name	Comments
P1	P1	Amplitude scaling factor.
P2	P2	
P3	A0	Constant background offset.
P4	A2	Linear background correction term.
P5	A3	Quadratic background correction term.

Remarks

When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

Ftn 0019: Complementary Incomplete Gamma Function (GammaQ) With Background Correction



Equation

The incomplete gamma function, GammaP, is defined as:

$$\mathrm{GammaQ}(a,x) = 1 - \mathrm{GammaP}(a,x) = \frac{1}{\Gamma(a)} \int_x^{\infty} e^{-t}\, e^{a-1}\, dt$$

There are four variations of this function:

- $Y = P1 * \mathrm{GammaQ}(P2, X)$
- $Y = P1 * \mathrm{GammaQ}(P2, X) + P3$
- $Y = P1 * \mathrm{GammaQ}(P2, X) + P3 + P4 * X$
- $Y = P1 * \mathrm{GammaQ}(P2, X) + P3 + P4 * X + P5 * X^2$

in which:

- Y is the measured response.
- X is the independent variable.

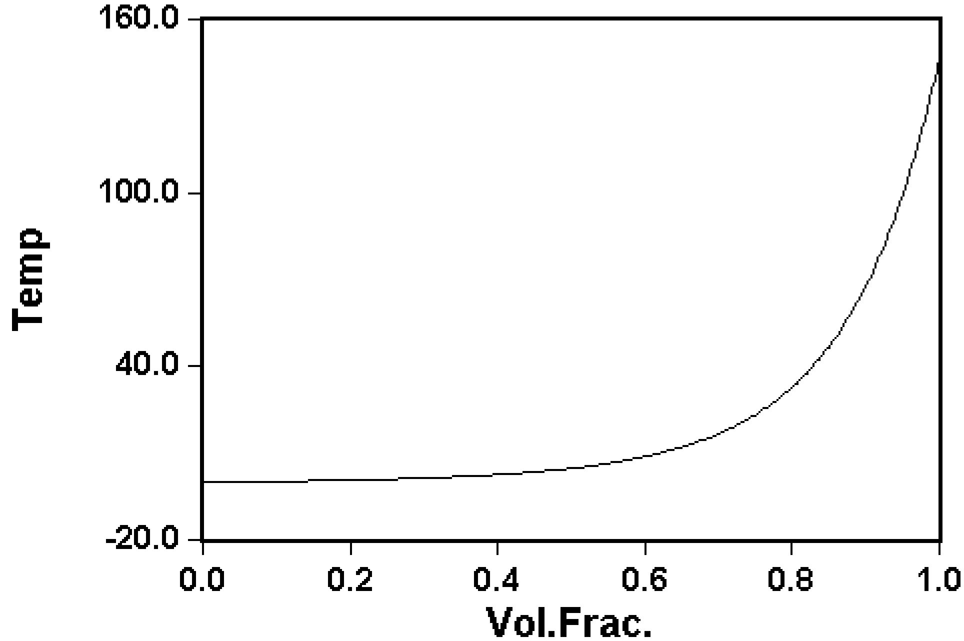
Parameters

Parameter	Name	Comments
P1	P1	Amplitude scaling factor.
P2	P2	
P3	A0	Constant background offset.
P4	A2	Linear background correction term.
P5	A3	Quadratic background correction term.

Remarks

When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

Ftn 0020: Boiling Curve_1



Equation

$$Y = e^{\left[P1 * X^{K1} + P2 * X^{K2}\right]} - 1$$

in which:

- Y is the measured response, often the temperature.
- X is the independent variable, often the volume fraction.

Constants

Constant	Name	Comments
K1	K1	Default value is 1.0
K2	K2	Default value is 2.0

Parameters

Parameter	Name	Comments
P1	P1	

Parameter	Name	Comments
P2	P2	

Sample Applications

- Correlating the boiling temperature, Y, with the volume fraction, X, of solvent in petroleum product mixtures.

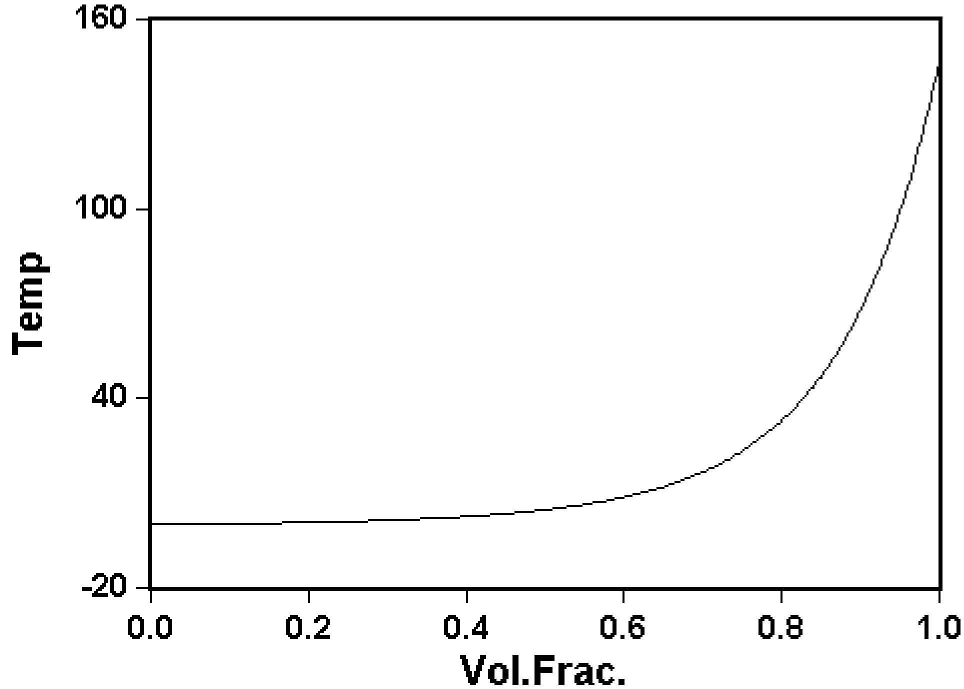
Remarks

When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

Also see

Function 0021 46

Ftn 0021: Boiling Curve_2



Equation

$$Y = e^{\left[P1 * X^{P3} + P2 * X^{P4}\right]} - 1$$

in which:

- Y is the measured response, often the temperature.
- X is the independent variable, often the volume fraction.

Parameters

Parameter	**Name**	**Comments**
P1	P1	
P2	P2	
P3	P3	
P4	P4	

Sample Applications

- Correlating the boiling temperature, Y, with the volume fraction, X, of solvent in petroleum product mixtures.

Remarks

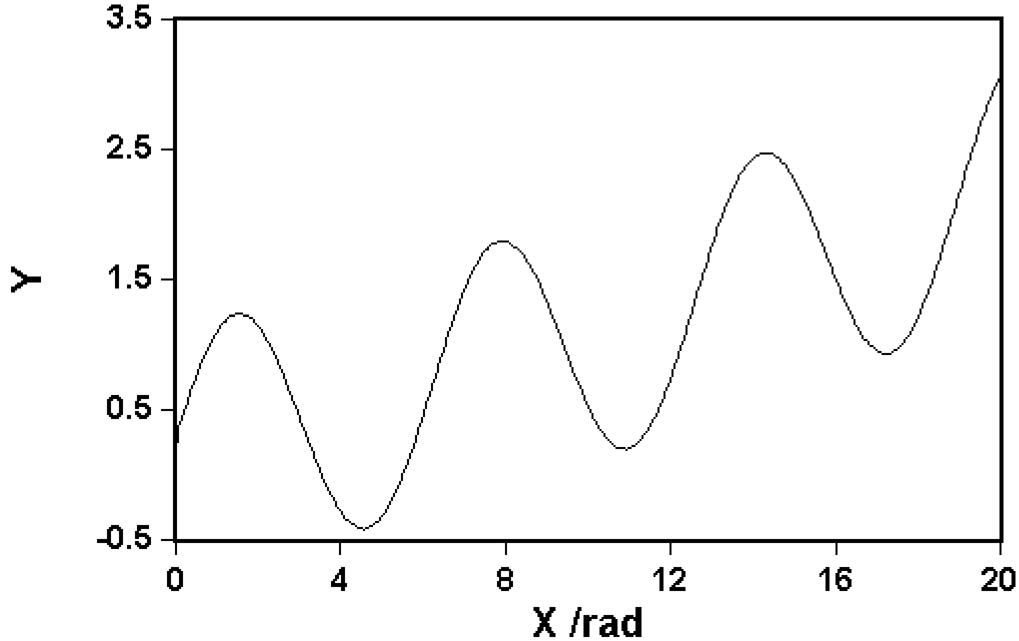
Because of the extreme non linearity of the function, ***FitAll*** may arrive at one of several possible solutions. Manual adjustment of the initial estimates will most likely be necessary.

When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

Also see

Function 0020 44

Ftn 0022: Sine With Background Correction



Equation

The general form of the function is:

$$Y = P1 * \mathrm{Sin}(P2 * X + P3) + \sum_i Ai * X^i$$

in which:

- Y is the measured response.
- X is the independent variable, the angle in radians.

Parameters

Parameter	**Name**	**Comments**
P1	Ampl	Amplitude of the sine.
P2	B	
P3	Phi	Phase shift (in radians).
P4	A0	Constant background offset.
P5	A1	Linear background correction term.

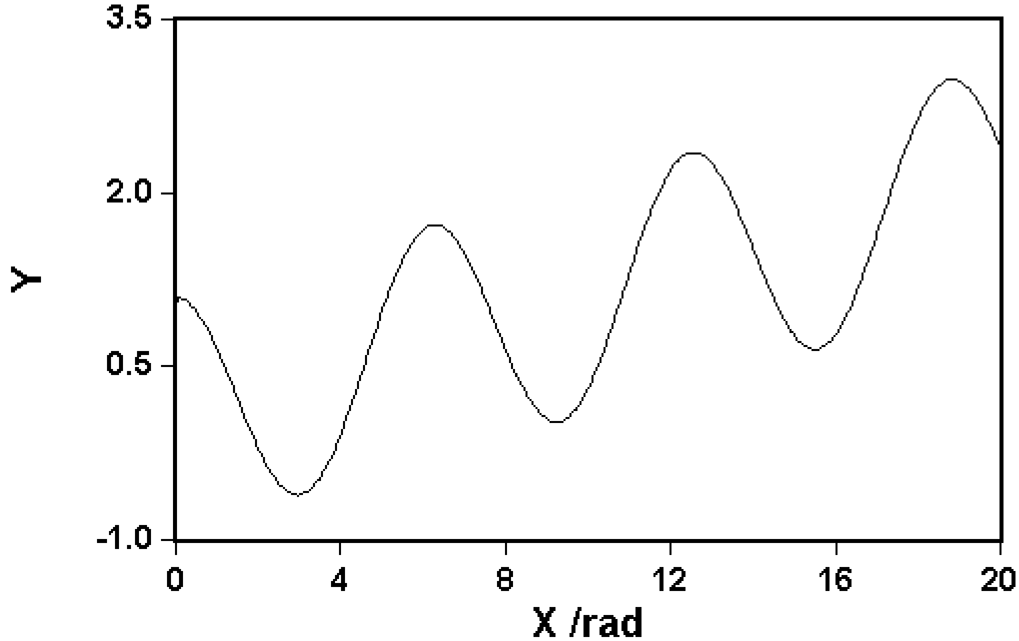
Parameter	Name	Comments
P6	A2	Quadratic background correction term.

Remarks

FitAll's automatic initial estimate procedure assumes that the data will cover at least one and a half complete cycles.

The Edit, data Modify... menu choice can be used to convert angles to and from degrees and radians.

Ftn 0023: Cosine With Background Correction



Equation

The general form of the function is:

$$Y = P1 * Cos(P2 * X + P3) + \sum_i Ai * X^i$$

in which:

- Y is the measured response.
- X is the independent variable, the angle in radians.

Parameters

Parameter	Name	Comments
P1	Ampl	Amplitude of the cosine.
P2	B	
P3	Phi	Phase shift (in radians).
P4	A0	Constant background offset.
P5	A1	Linear background correction term.

Parameter	Name	Comments
P6	A2	Quadratic background correction term.

Remarks

FitAll's automatic initial estimate procedure assumes that the data will cover at least one and a half complete cycles.

The Edit, data Modify... menu choice can be used to convert angles to and from degrees and radians.

Ftn 0024: Multiple Linear_2: Y = ∑(Pj*Xj,k[j])

Equation

The general form of the function is:

$$Y = \sum_j P_j * X_{i,K[j]}$$

For example:

- Y = P1*X1 {a straight line with zero intercept}
- Y = P1*X1 + P2*X2
- Y = P1*X1 + P2*X5
- Y = P1*X3 + P2*X5 + P3*X7

in which:

- Y is the measured response.
- X is the independent variable.

Constants

Constant	Name	Comments
K1	K1	Mapping constant for parameter P1 that identifies the independent variable that is multiplied by parameter P1. For example, if K1 = 3 then the equation would be Y = P1*X3
K2	K2	Mapping constant for parameter P2.
K3	K3	Mapping constant for parameter P3.
etc.	etc.	etc.

Parameters

Parameter	Name	Comments
P1	P1	First parameter is a multiplier of the independent variable identified by constant K1.

Parameter	Name	Comments
P2	P2	Second parameter is a multiplier of the independent variable identified by constant K2.
P3	P3	Third parameter is a multiplier of the independent variable identified by constant K3.
etc.	etc.	etc.

Multi-Fits

Function 0024 is Multi-Fit enabled.

This means that:

Variations of this function in which the number of parameters, P, is less than or equal to the number of independent variables, X, in the data set can be analyzed at once.

NOTE:
The number of configurations that will be generated can be calculated using the formula:

Number of Configs = (Total Num. of independent variables)! / (Number of parameters)! * ((Total Num. of independent variables) - (Number of parameters))!, in which "!" is the "factorial" operator.

For the F0024TST01.DTA data file, which has six (6) independent variables and a setup with three (3) parameters there will be (6!)/((3!)*(6-3)!) configurations. That is, 20 configurations will be generated.

Although the contents of the '.fmc' file can be viewed with text editors such as NotePad and TextPad, it is most unlikely that you will find this to be a useful endeavour.

To do the Multi-Fit analysis:

- Retrieve the data set with more than one independent variable; for example, F0024TST01.DTA.

- Select the menu items Edit, Generate Multi-Fit configs....

  In the dialog box that appears, choose F0024 with three (3) parameters and an appropriate name for the "configuration file" that will be created.

  Click the **OK** button to create the configuration file.

- Select the menu items Analyze, SetUp....

  In the dialog box that appears:

  On the Function page: Select function 0024 with three (3) parameter and the analysis type of 'Multi-Fit'

On the Multi-Fit page: Set the 'Config. File Name' and the 'Results File Name'. as well as any other items that you like.

- Select the menu items: Analyze, Analyze to do the analyses. The results will be saved to the Results file.

Sample Applications

- Determining the factors (independent variables) that are most important in calculating the assessed value of a real estate property.

  Many factors (independent variables) can contribute to the assessed value of a property. For example: location, lot size, lot frontage, floor area, number of bathrooms, number of bedrooms, number of stories, parking arrangements (such as, street parking, car port, garage, attached garage), proximity to schools, distance from mass transit, types of mass transit, etc. are all potential contributors to the assessed value.

  It is reasonable to assume that not all of the independent variables, factors, are independent of one another.

  Under such circumstances, a regression analysis that includes all of the independent variables will result in a fit in which the standard deviation of some of the parameters is large, indicating that those particular independent variables are not statistically significant in determining the calculated value.

  However, it is a characteristic of least squares regression analysis that it may be somewhat arbitrary in assigning the errors associated with the resolved parameters that are not actually independent of one another.

  One way to get around this issue is to assume that only some of the independent variables are truly independent and to fit the data to every possible form (variation) of the equation which has fewer parameters than there are independent variables.

- Correlating the relationship between the number and positions of substituents in a series of related chemicals with the rate (or log rate) of a chemical reaction.

Remarks

Initial estimates are not required for this function because it is linear in its parameters.

A 'constant' term can be introduced into the function by creating a data column in which all of its values are one, 1.0.

The configurations of this function are distinguished from one another by the values of the constants, K.

For example, in a data set containing eight columns, the first six columns contain the values of the independent variables X1 to X6.

Configurations containing from one to six constants, K, will be generated. Some of the configurations are shown below:

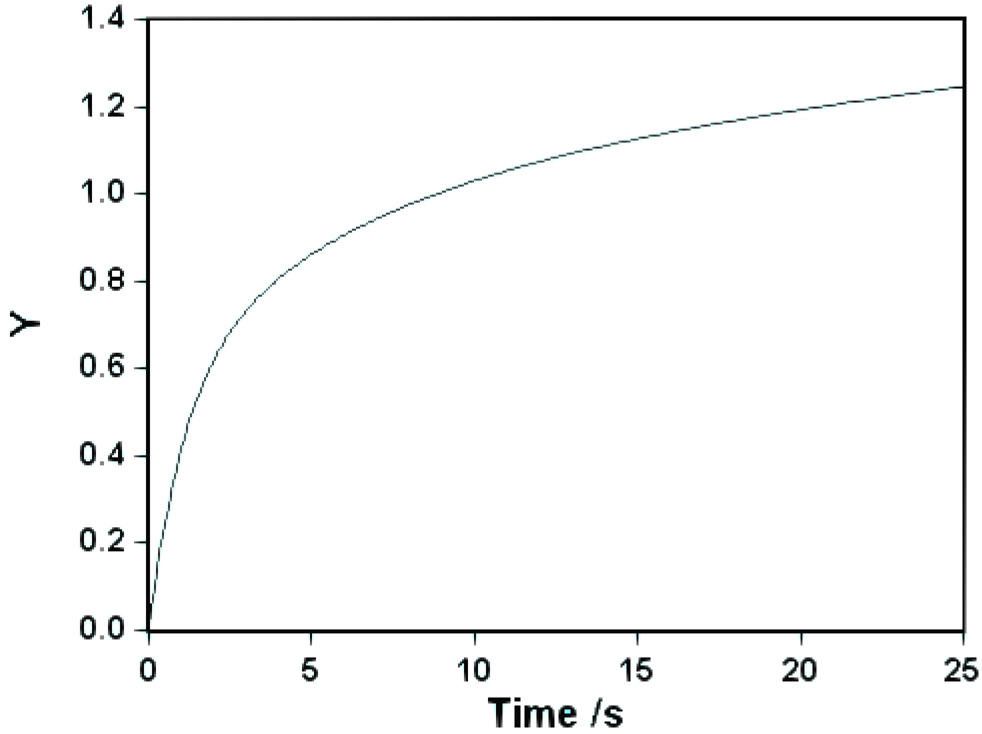
Config#	K1	K2	K3	K4	K5	K6	Resulting Equation: Y =
1	1	0	0	0	0	0	P1*X1
2	2	0	0	0	0	0	P1*X2
3	3	0	0	0	0	0	P1*X3
etc.	etc.	etc.	etc.	etc.	etc.	etc.	etc.
7	1	2	0	0	0	0	P1*X1 + P2*X2
8	1	3	0	0	0	0	P1*X1 + P2*X3
9	1	4	0	0	0	0	P1*X1 + P2*X4
etc.	etc.	etc.	etc.	etc.	etc.	etc.	etc.
22	1	2	3	0	0	0	P1*X1 + P2*X2 + P3*X3
23	1	2	4	0	0	0	P1*X1 + P2*X2 + P3*X4
24	1	2	5	0	0	0	P1*X1 + P2*X2 + P3*X5
etc.	etc.	etc.	etc.	etc.	etc.	etc.	etc.
63	1	2	3	4	5	6	P1*X1 + P2*X2 + P3*X3 + P4*X4 + P5*X5 + P6*X6

Also see

Function 0008: Multiple Linear 20

How to do Multi-Fit Analyses in the FitAll Reference Guide

Ftn 0025: Y = P[1] * X + ∑(P[2j] * (1 - exp(-P[2j+1] * X)))



Equation

This function has two general forms:

$$Y = P_1 * X + \sum_{j=1}^{n} \left[P_{2j} * \left(1 - e^{-P_{2j+1} * X} \right) \right]$$

and

$$Y = P_1 * (X - Xo) + \sum_{j=1}^{n} \left[P_{2j} * \left(1 - e^{-P_{2j+1} * (X - Xo)} \right) \right]$$

in which:

- Y is the measured response.
- X is the independent variable, often the time in seconds.
- Xo is a parameter that corrects for small determinate errors in X.
- n is the number of exponentials and can have values from 1 to 50.

This function has 20 variations. For example:

- $$Y = P_1 * X + P_2 * \left(1 - e^{-P_3 * X}\right)$$
- $$Y = P_1 * X + P_2 * \left(1 - e^{-P_3 * X}\right) + P_4 * \left(1 - e^{-P_5 * X}\right)$$
- $$Y = P_1 * (X - Xo) + P_2 * \left(1 - e^{-P_3 * (X - Xo)}\right)$$

Parameters

Parameter	**Name**	**Comments**
P1	Ao	Slope of a "background drift".
P2	A1	Amplitude of the first exponential
P3	B1	Rate constant or 1/(time constant), 1/τ, for the first exponential.
P4	A2	Amplitude of the second exponential
P5	B2	Rate constant or 1/(time constant), 1/τ, for the second exponential.
etc.	etc.	
Pmax - 1	A(2j-1)	Amplitude of the last exponential
Pjmax	B(2j)	Rate constant or 1/(time constant), 1/τ, for the last exponential.
Pmax + 1	Xo	Xo offset. In many experiments there may be a small offset in the value of X caused by, for example, an instrument calibration error. With exponential functions such determinate errors, even though very small, may cause a dramatic reduction in the quality of the fit. Including this parameter *may* improve the quality of the fit.

Sample Applications

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Remarks

When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

When the function contains more than one exponential term, ***FitAll*** will attempt to provide initial parameter estimates; however, these initial estimates are not very reliable and it is almost certain that you will have to manually adjust them before you do the fit.

Often the best fitting strategy is to:

1. Fit the first part of the data with one exponential term in the function. Let ***FitAll*** make the initial parameter estimates.

2. Fit a larger segment of the data with two exponential terms in the function. In this case, manually provide the required initial parameter estimate by using the results of the first analysis and making reasonable guesses for the remaining parameters.

If you suspect that there is an Xoffset the best fitting strategy is to:

1. Fit the data without the Xoffset parameter.

2. Choose Analyze, Setup and select the same function, but this time include the Xoffest parameter.

3. In the Parameters Tab of the Setup dialog set the initial estimate of the Xoffset paramter to 0, zero. Do NOT click the Automatic Estimates button. By doing this, the initial estimates of all of the other parameters will have the values that were determined in the earlier fit.

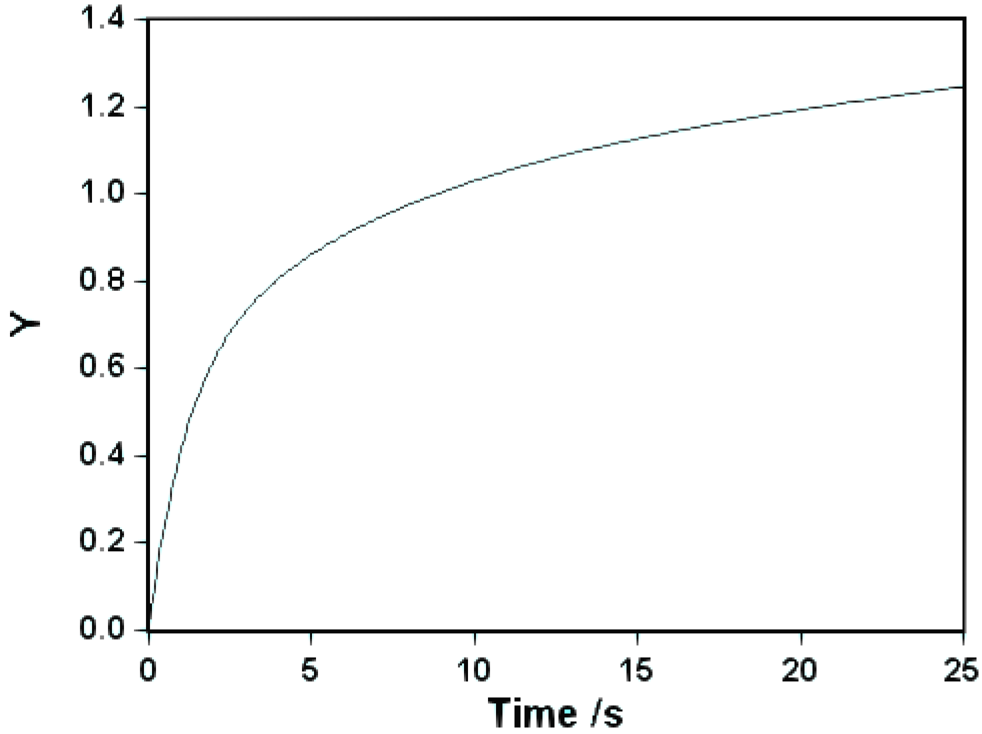
Also see

Function 0026 59

Function 0001 3

Function 0002 6

Ftn 0026: Y = ∑(P[2j-1] * (1 - exp(-P[2j] * X)))



Equation

This function has two general forms:

$$Y = \sum_{j=1}^{n} \left[P_{2j-1} * \left(1 - e^{-P_{2j} * X} \right) \right]$$

and

$$Y = \sum_{j=1}^{n} \left[P_{2j-1} * \left(1 - e^{-P_{2j} * (X - Xo)} \right) \right]$$

in which:

- Y is the measured response.
- X is the independent variable, often the time in seconds.
- Xo is a parameter that corrects for small determinate errors in X.
- n is the number of exponentials and can have values from 1 to 50.

This function has 20 variations. For example:

- $$Y = P_1 * \left(1 - e^{-P_2 * X}\right)$$
- $$Y = P_1 * \left(1 - e^{-P_2 * (X - Xo)}\right)$$
- $$Y = P_1 * \left(1 - e^{-P_2 * X}\right) + P_3 * \left(1 - e^{-P_4 * X}\right)$$

Parameters

Parameter	**Name**	**Comments**
P1	A1	Amplitude of the first exponential
P2	B1	Rate constant or 1/(time constant), 1/τ, for the first exponential.
P3	A2	Amplitude of the second exponential
P4	B2	Rate constant or 1/(time constant), 1/τ, for the second exponential.
etc.	etc.	
Pmax - 1	A(2j-1)	Amplitude of the last exponential
Pmax	B(2j)	Rate constant or 1/(time constant), 1/τ, for the last exponential.
Pmax + 1	Xo	Xo offset. In many experiments there may be a small offset in the value of X caused by, for example, an instrument calibration error. With exponential functions such determinate errors, even though very small, may cause a dramatic reduction in the quality of the fit. Including this parameter *may* improve the quality of the fit.

Sample Applications

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Remarks

When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

When the function contains more than one exponential term, ***FitAll*** will attempt to provide initial parameter estimates; however, these initial estimates are not very reliable and it is almost certain that you will have to manually adjust them before you do the fit.

Often the best fitting strategy is to:

1. Fit the first part of the data with one exponential term in the function. Let ***FitAll*** make the initial parameter estimates.

2. Fit a larger segment of the data with two exponential terms in the function. In this case, manually provide the required initial parameter estimate by using the results of the first analysis and making reasonable guesses for the remaining parameters.

If you suspect that there is an Xoffset the best fitting strategy is to:

1. Fit the data without the Xoffset parameter.

2. Choose Analyze, Setup and select the same function, but this time include the Xoffest parameter.

3. In the Parameters dialog page set the initial estimate of the Xoffset paramter to 0, zero. Do NOT click the Automatic Estimates button. By doing this, the initial estimates of all of the other parameters will have the values that were determined in the earlier fit.

Also see

Function 0025 56

Function 0001 3

Function 0002 6

Appendix

Getting Help

To get technical or other assistance from MTR Software you can:

Visit MTR Software's website at:

www.fitall.com

Email MTR Software at:

support@fitall.com

Write to MTR Software at:

MTR Software

77 Carlton Street, Suite 808

Toronto ON Canada

M5B 2J7

Telephone MTR Software at:

416-596-1499

Describe your problem or difficulty as completely as you can. We will try to answer your query quickly and completely.

You should also include your email address as well as your daytime, evening and weekend telephone numbers.

Adding Functions to FitAll

There are four ways to add your own specialized functions to ***FitAll***.

1. In ***FitAll*** version 10 you can use the new "Scripted Function" feature to add functions that can be defined by a one-line expression and contains one independent variable, X. and up to ten parameters, P.

2. You can contact ***MTR*** **Software** to get a quotation on the cost of creating a custom ***FitAll*** **Function Library** for you.

3. The ***FitAll*** **Programmer's Guide**, which is included with ***FitAll*** **Research Edition**, explains:

   - how to modify the supplied source code for the User Defined ***FitAll*** **Function Libraries** and

   - how to compile them using Embarcadero / CodeGear / Borland Delphi version 5 to XE2, **FreePascal** version 2.2 or later and **Lazarus** version 1.0 or later. FreePascal and Lazarus are open source Pascal compilers available from www.freepascal.org and www.lazarus.freepascal.org . Lazarus is highly recommended.

4. You can contact ***MTR*** **Software** and request that the function be added to one of ***FitAll***'s **Function Libraries**.

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