Version 7

FitAll

nonlinear regression analysis

Peaks Function Guide

Published by

MTR Software

77 Carlton Street, Suite 808
Toronto ON Canada
M5B 2J7

www.fitall.com

support@fitall.com

416-596-1499

Contents

THIS IS AN INTENTIONALLY EMPTY PAGE

Introduction

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

THIS IS AN INTENTIONALLY EMPTY PAGE

Function Reference Overview

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

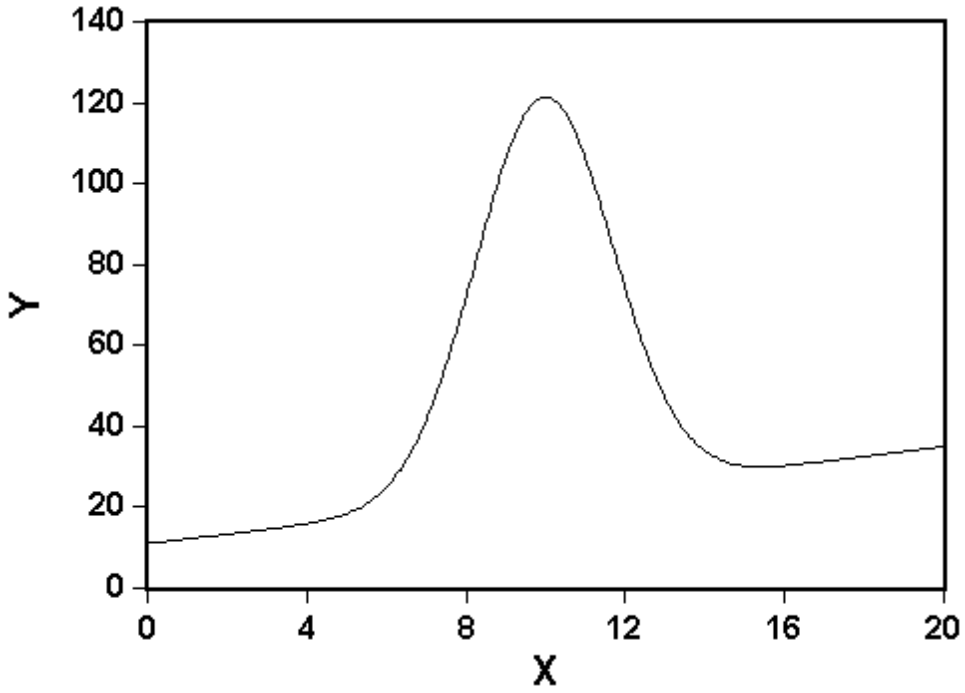
Remarks

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 0301: Gaussian With Background Correction



Equation

$$Y = P1 * e^{\left[-2.77 * \left(\frac{(X - P2)}{P3}\right)^2\right]} + \sum_{i=0} Ai * X^i$$

Four variations of the function are available, for example:

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

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.

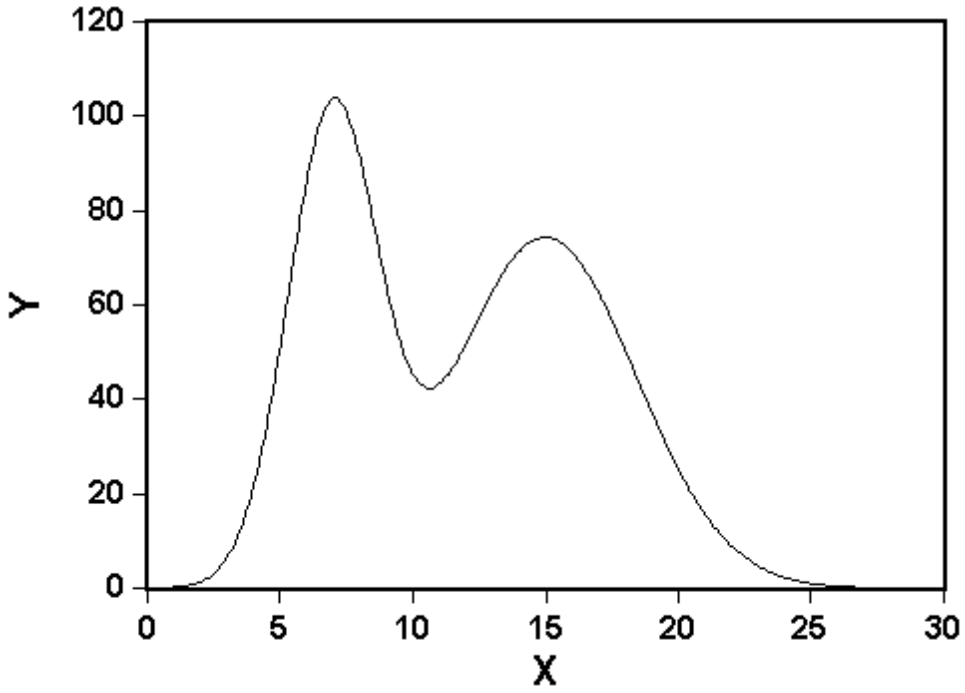
Sample Applications

- 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 0302: Sum of Gaussians With Background Correction



Equation

The general form of the function is:

$$Y = \sum_{i=1}^{n} \left(P_{3i-2} * e^{\left[-2.77 * \left(\frac{X - P_{3i-1}}{P_{3i}} \right)^2 \right]} \right) + \sum_{j=0}^{n2} \left(P_{3n+1+j} * X^j \right)$$

in which:

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

For example:

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

- $$Y = P1 * e^{\left[-2.77*\left(\frac{(X - P2)}{P3}\right)^2\right]} + P4 + P5 * X + P6 * X^2$$
- $$Y = P1 * e^{\left[-2.77*\left(\frac{X - P2}{P3}\right)^2\right]} + P4 * e^{\left[-2.77*\left(\frac{X - P5}{P6}\right)^2\right]}$$
- $$Y = P1 * e^{\left[-2.77*\left(\frac{X - P2}{P3}\right)^2\right]} + P4 * e^{\left[-2.77*\left(\frac{X - P5}{P6}\right)^2\right]} + P7 * e^{\left[-2.77*\left(\frac{X - P8}{P9}\right)^2\right]}$$

Parameters

Parameter	Name	Comments
P1	Ypeak1	Maximum value of Y for the first Gaussian curve.
P2	Xpeak1	Value of X when Y = Ypeak1.
P3	FWHH1	Full-Width at Half-Height for the first Gaussian curve. Width of the curve at Y = Ypeak1/2.
P4	Ypeak2	Maximum value of Y for the second Gaussian curve.
P5	Xpeak2	Value of X when Y = Ypeak2.
P6	FWHH2	Full-Width at Half-Height for the second Gaussian curve. Width of the curve at Y = Ypeak2/2.
P7	Ypeak3	Maximum value of Y for the second Gaussian curve.
etc.	etc.	etc.
	A0	Constant background offset.
	A1	Linear background correction term.
	A2	Quadratic background correction term.

Sample Applications

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

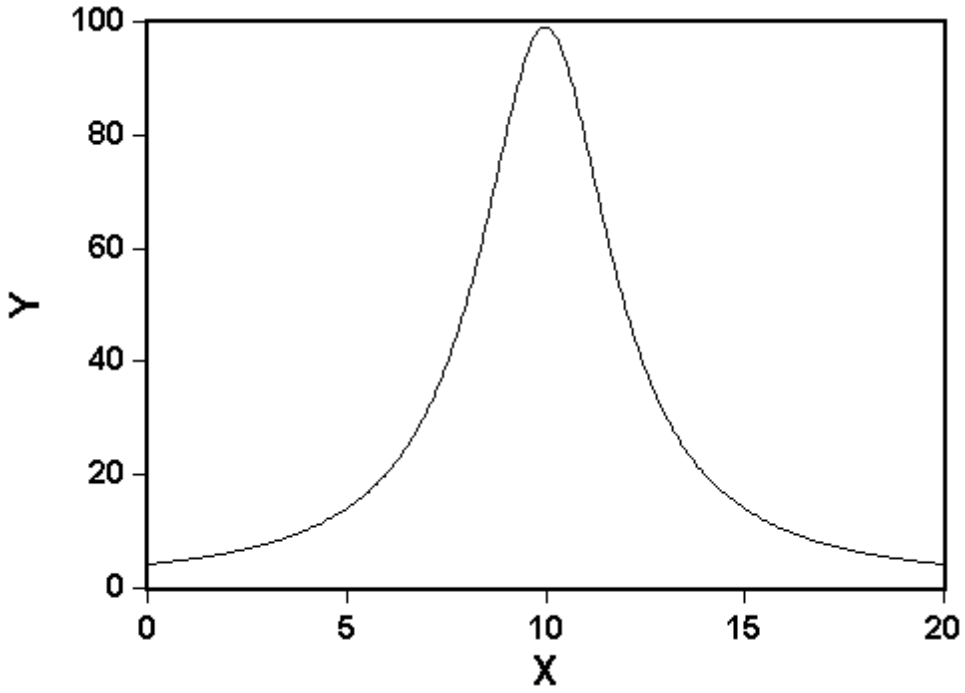
Remarks

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

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

Often the best fitting strategy is to fit only part of your data to one Gaussian curve, then fit a larger segment of the data to the sum of two Gaussians, etc., until all of your data are included in the analysis.

Ftn 0303: Lorentzian With Background Correction



Equation

$$Y = \frac{P1 * P3^2}{\left[4 * (X - P2)^2 + P3^2\right]} + \sum_i Ai * X^i$$

For example:

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

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.

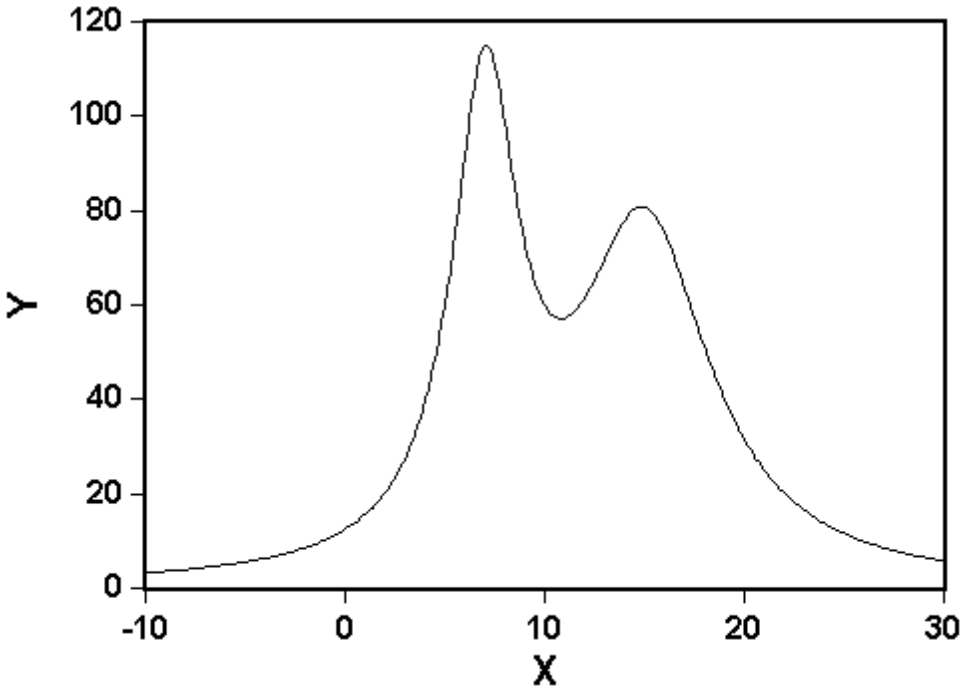
Sample Applications

- 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 0304: Sum of Lorentzians With Background Correction



Equation

The general form of the function is:

$$Y = \sum_{i=1}^{n} \left(\frac{P_{3i-2} * P_{3i}^2}{\left[4 * (X - P_{3i-1})^2 + P_{3i}^2 \right]} \right) + \sum_{j=0}^{n2} \left(P_{3n+1+j} * X^j \right)$$

in which:

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

For example:

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

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

Parameters

Parameter	Name	Comments
P1	Ypeak1	Maximum value of Y for the first Lorentzian curve.
P2	Xpeak1	Value of X when Y = Ypeak1.
P3	FWHH!	Full-Width at Half-Height for the first Lorentzian curve. Width of the curve at Y = Ypeak1/2.
P4	Ypeak2	Maximum value of Y for the second Lorentzian curve.
P5	Xpeak2	Value of X when Y = Ypeak2.
P6	FWHH2	Full-Width at Half-Height for the second Lorentzian curve. Width of the curve at Y = Ypeak2/2.
P7	Ypeak3	Maximum value of Y for the second Lorentzian curve.
etc.	etc.	etc.
	A0	Constant background offset.
	A1	Linear background correction term.
	A2	Quadratic background correction term.

Sample Applications

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

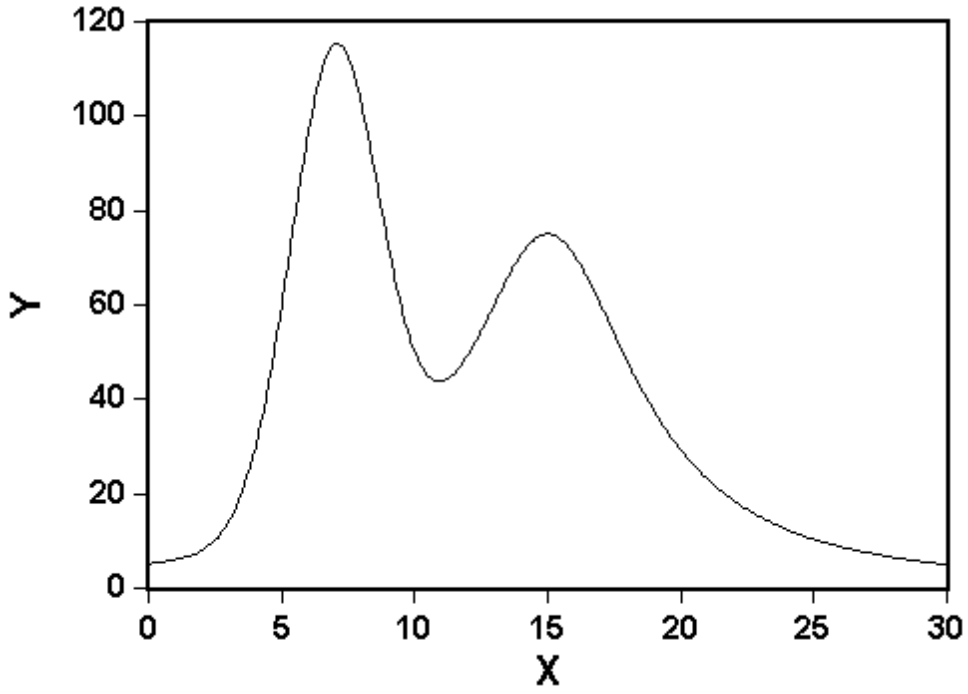
Remarks

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

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

Often the best fitting strategy is to fit only part of your data to one Lorentzian curve, then fit a larger segment of the data to the sum of two Lorentzians, etc., until all of your data are included in the analysis.

Ftn 0305: Sum of Gaussians and Lorentzians With Background Correction



Equation

Y is the sum of one to five Gaussian and Lorentzian curves. That is, the total number of Gaussians plus Lorentzians is limited to five.

The simplest form of the function is:

$$Y = P1 * e^{\left[-2.77*\left(\frac{X - P2}{P3}\right)^2\right]} + \frac{P4 * P6^2}{[4 * (X - P5)^2 + P6^2]}$$

in which:

- Y is the measured response.
- X is the independent variable.
- All forms of the above may also have a background correction polynomial of up to three terms, that is, a quadratic polynomial.

Parameters

Parameter	Name	Comments
P1	YpeakG1	Maximum value of Y for the first Gaussian curve.
P2	XpeakG1	Value of X when Y = YpeakG1.
P3	FWHHG1	Full-Width at Half-Height for the first Gaussian curve. Width of the curve at Y = Ypeak1 / 2.
P4	YpeakL1	Maximum value of Y for the first Lorentzian curve.
P5	XpeakL1	Value of X when Y = YpeakL1.
P6	FWHHL1	Full-Width at Half-Height for the first Lorentzian curve. Width of the curve at Y = YpeakL1 / 2.
P7	Ypeak3	Maximum value of Y for the second Lorentzian curve.
etc.	etc.	etc.
	A0	Constant background offset.
	A1	Linear background correction term.
	A2	Quadratic background correction term.

Sample Applications

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

Remarks

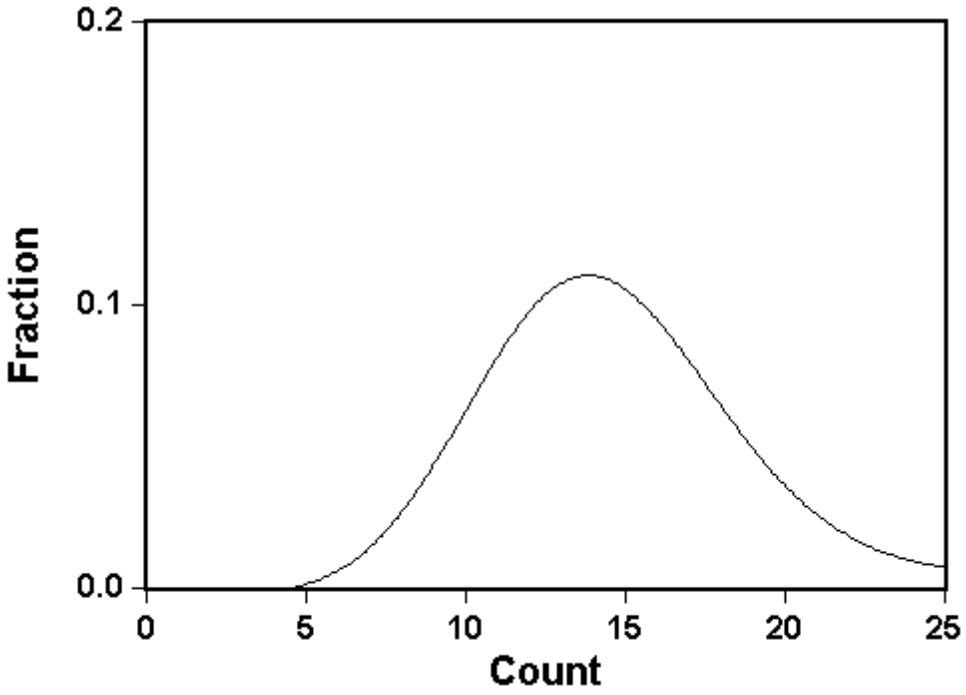
When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

FitAll will calculate only some of the required initial estimates - those for the first Gaussian and the background polynomial correction terms.

FitAll assumes that the first part of the data will correspond to the first Gaussian rather than to the first Lorentzian. The remaining initial parameter estimates must be entered manually.

Often the best fitting strategy is to fit only part of your data to one Gaussian curve or to one Lorentzian curve , then fit a larger segment of the data to the sum of two Gaussians, etc., until all of your data are included in the analysis.

Ftn 0306: Poisson With Background Correction



Equation

$$Y = P2 * e^{[X*Ln(P1)-P1-Ln(X!)]} + \sum_{i=0}^{n} \left(A_i * X^i\right)$$

For example:

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

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. The standard deviation of a Poisson distribution is equal to

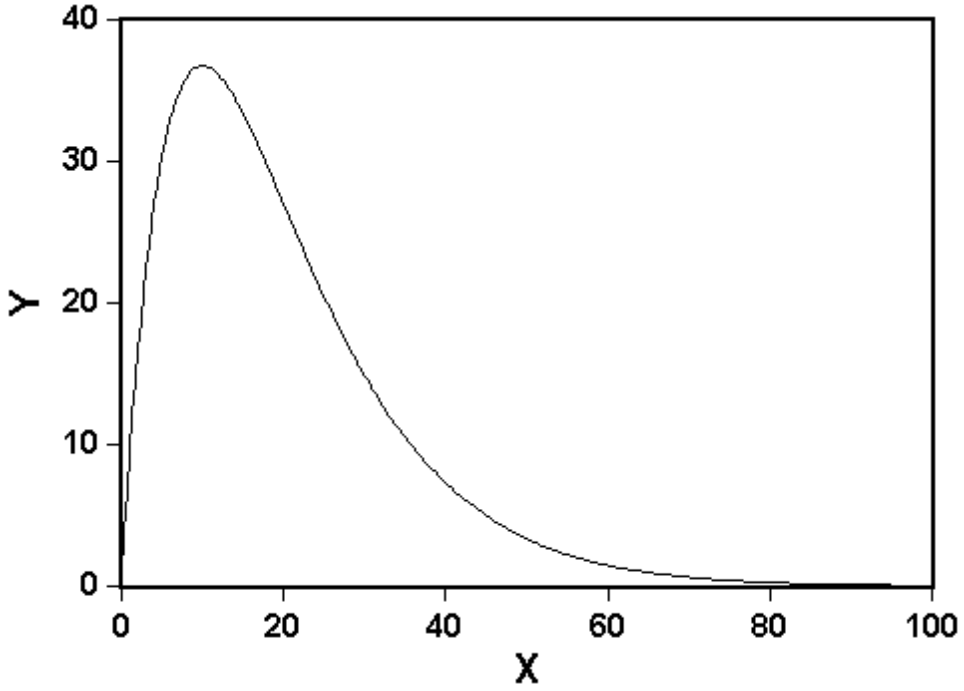
Parameter	Name	Comments
		the square root of the mean.
P2	NF	Normalization Factor. Amplitude scaling factor, such that Sum{Yi}/P2 = 1.0. If the Y-values correspond to the probability of observing X events per unit time, P2 should have a value of 1.
P3	A0	Constant background offset.
P4	A1	Linear background 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 0307: Impulse: Linear or Exponential Growth Coupled with Exponential Decay



Equation

The general form of the function is:

$$Y = P1*(X - P3)^{P4} * e^{\left[-P2*K1*(X-P3)\right]} + \sum_{i=0}^{n} \left(A_i * X^i\right)$$

For example:

- $Y = P1 * X * e^{\left[-P2*K1*X\right]}$
- $Y = P1 * (X - P3) * e^{\left[-P2*K1*(X-P3)\right]}$
- $Y = P1 * (X - P3)^{P4} * e^{\left[-P2*K1*(X-P3)\right]}$

in which:

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

Constants

Constant	Name	Comments
K1	K1	Arbitrary constant. Default value is 1.0.

Parameters

Parameter	Name	Comments
P1	P1	Amplitude of the exponential term.
P2	P2	Rate constant or 1/(time constant) for the exponential decay.
P3	P3	X offset (time zero offset). In the first two forms of the function P3 is assumed to be zero.
P4	P4	Growth order parameter. In the first two functions P4 is 1.0; that is, first order growth is assumed.
	A0	Constant background offset.
	A1	Linear background correction term.
	A2	Quadratic background correction term.

Sample Applications

- Describes an "impulse", such as that encountered when adding a "slug" of reagent to a chemical reactor in which mixing is not instantaneous.
- Describes the uptake and release of nutrients by biological systems.

Remarks

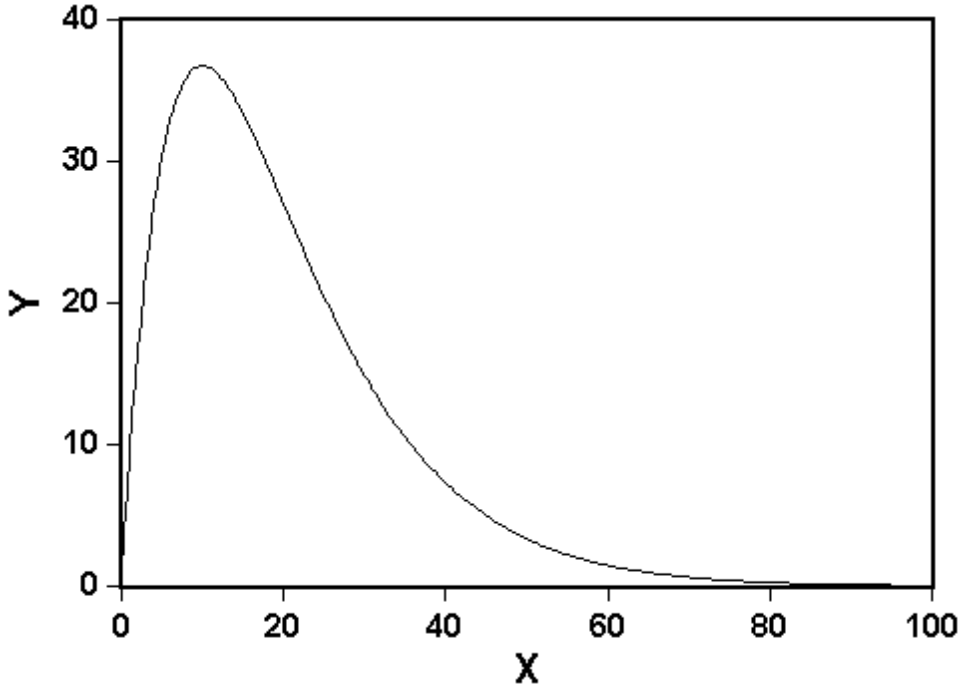
In the third form of the function, (X-P3) is assumed to be greater than zero (> 0).

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 0308 20

Ftn 0308: Impulse_2: Linear or Exponential Growth Coupled with Exponential Decay



Equation

The general form of the function is:

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

For example:

- $Y = P1 * X * e^{\left[-P2*K1*X\right]}$
- $Y = P1*X^{P3} *e^{\left[-P2*K1*X\right]}$

in which:

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

Constants

Constant	Name	Comments
K1	K1	Arbitrary constant. Default value is 1.0.

Parameters

Parameter	Name	Comments
P1	P1	Amplitude of the exponential term.
P2	P2	Rate constant or 1/(time constant) for the exponential decay.
P3	P3	Growth order parameter. In the first function first order growth is assumed.
	A0	Constant background offset.
	A1	Linear background correction term.
	A2	Quadratic background correction term.

Sample Applications

- Describes an "impulse", such as that encountered when adding a "slug" of reagent to a chemical reactor in which mixing is not instantaneous.
- Describes the uptake and release of nutrients by biological systems.

Remarks

In the third form of the function, (X-P3) is assumed to be greater than zero (> 0).

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 0307 17

THIS IS AN INTENTIONALLY EMPTY PAGE

Appendix

Getting Help

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

Visit MTR Software's website at:

www.fitall.com

and click on the menu selections

Support, ***FitAll* Forums**

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 three ways to add your own specialized functions to ***FitAll***.

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

2. 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, 6, 7, 2005, 2006, 2009 and 2010 or **FreePascal** version 2.2 and later, which is an open source Pascal compiler available from www.freepascal.org.

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

THIS IS AN INTENTIONALLY EMPTY PAGE

Index

- C -

- E -

- F -

- G -

- H -

- I -

- L -

- P -