*Version 9*

# FitAll

*nonlinear regression analysis*

## *Peaks Function Guide*

Published by

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# Contents

# 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**.

# 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.

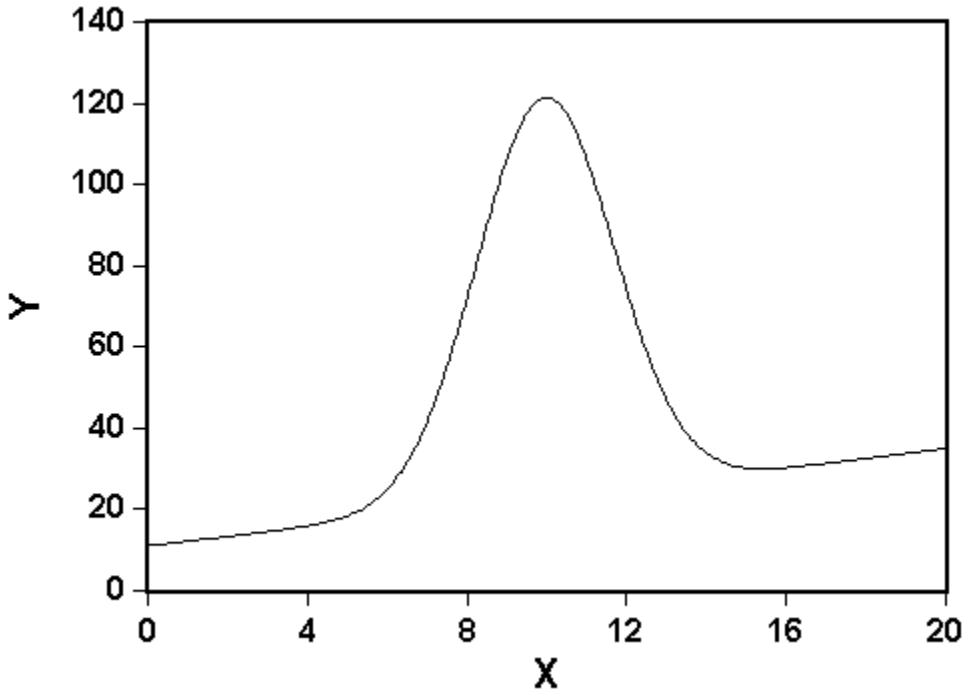
## *Remarks*

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.<br>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. |

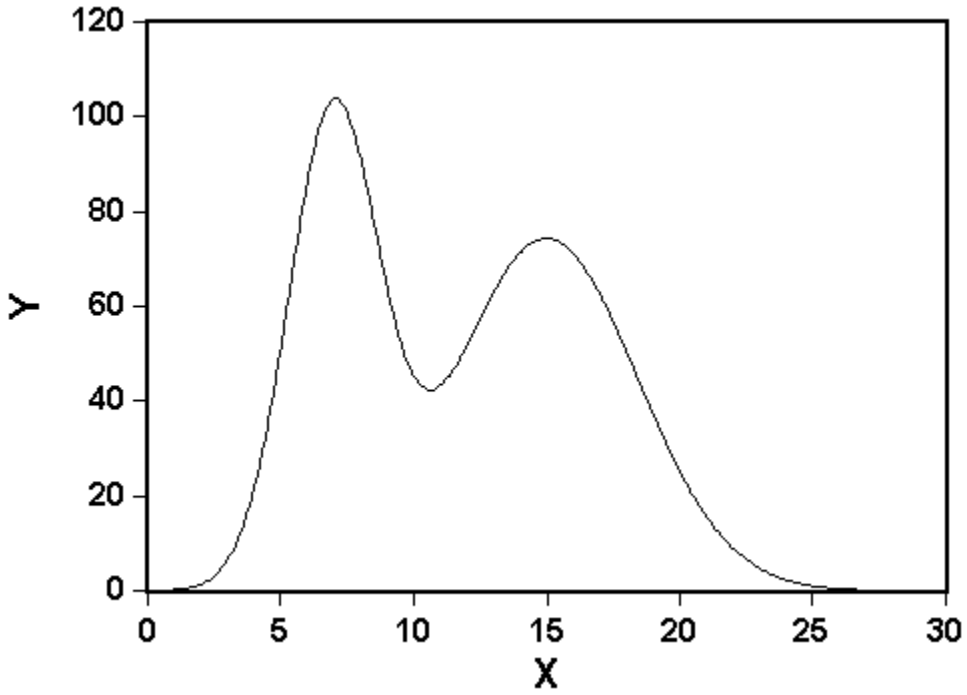
## Sample Applications

- 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.<br>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.<br>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.

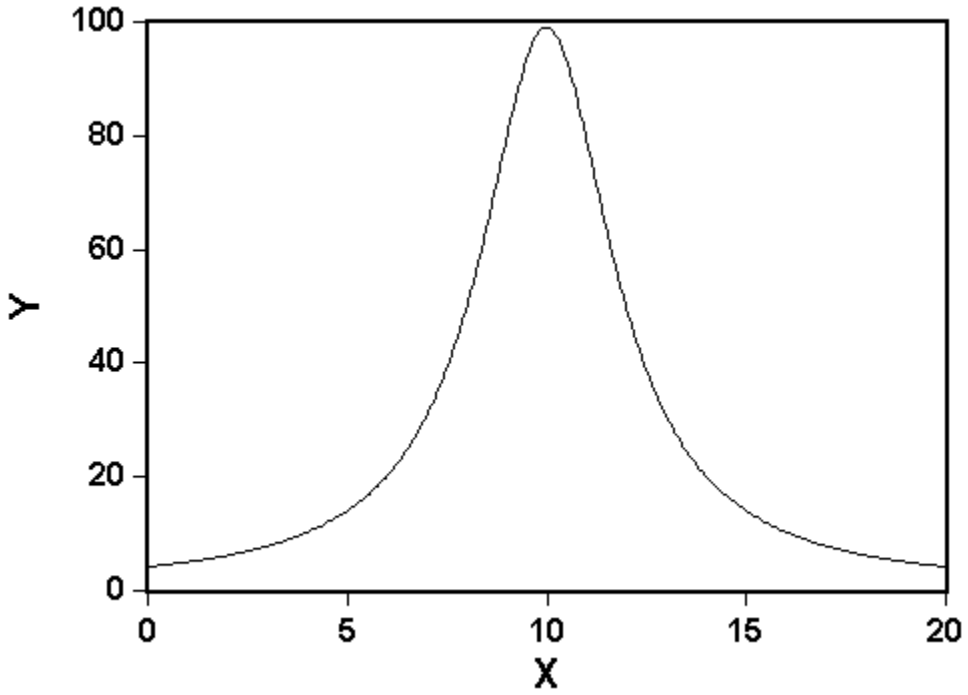
## Remarks

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.<br>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. |

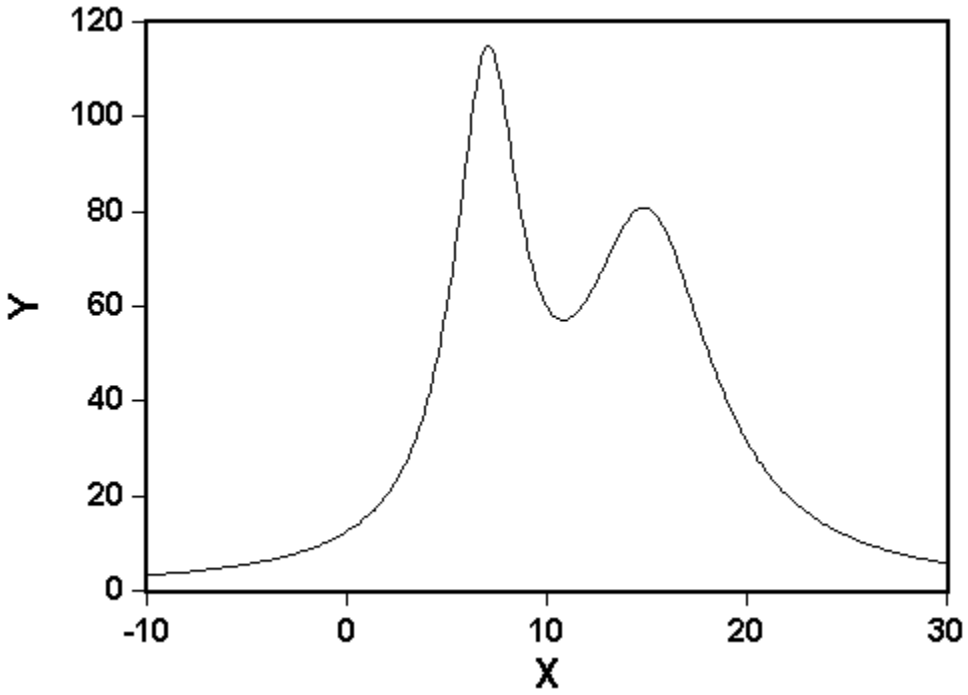
## Sample Applications

- 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.<br><br>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.<br><br>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.

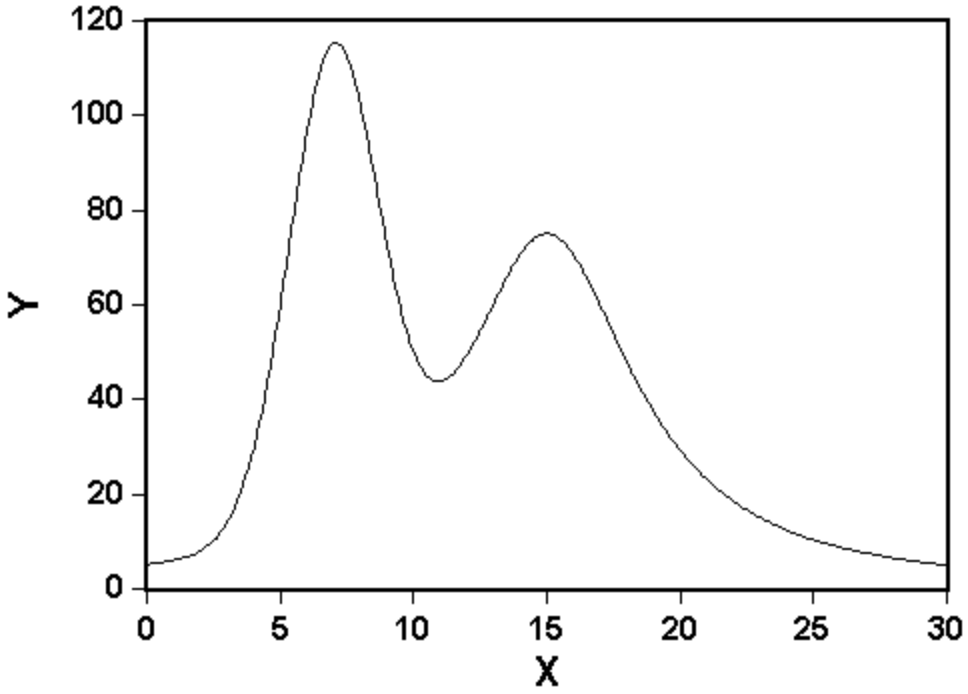
## Remarks

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.<br>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.<br>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

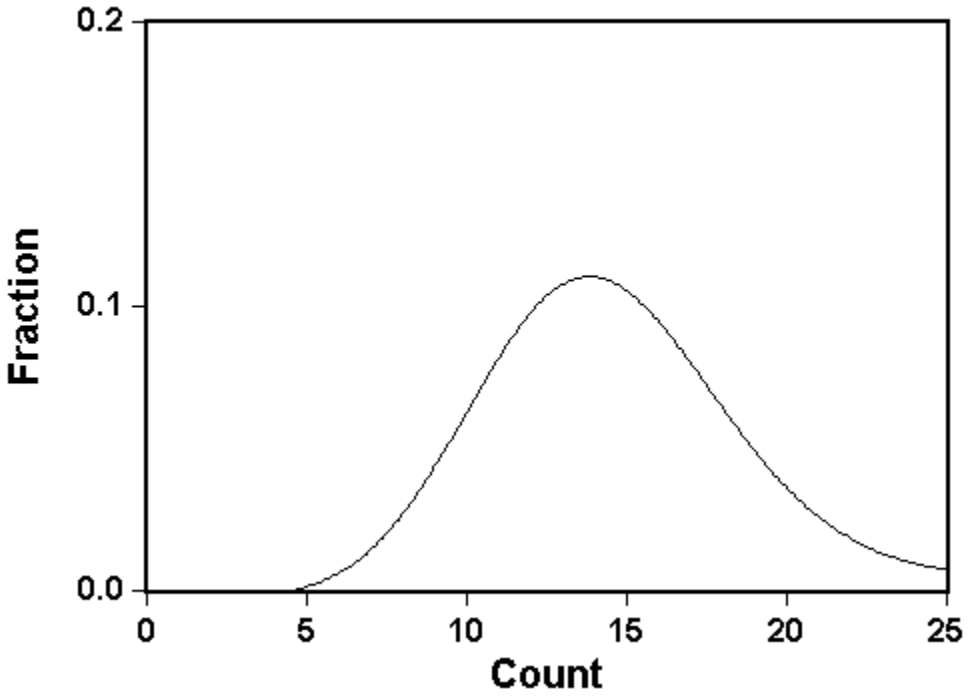
When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

***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 |

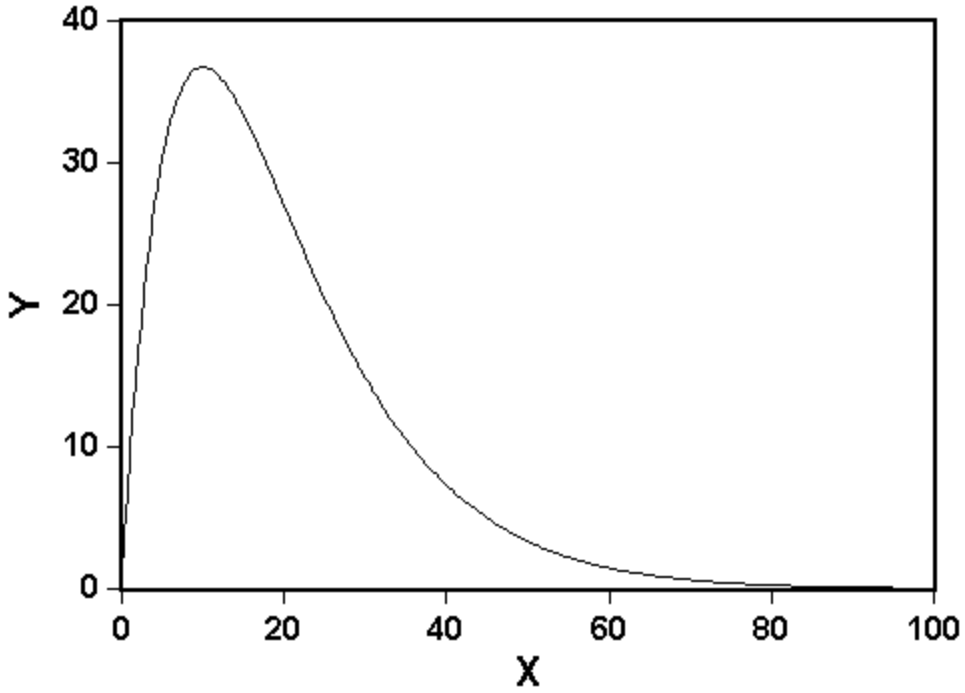
| Parameter | Name | Comments |
|---|---|---|
| | | equal to the square root of the mean. |
| P2 | NF | Normalization Factor.<br><br>Amplitude scaling factor, such that Sum{Yi}/P2 = 1.0.<br><br>If the Y-values correspond to the probability of observing X events per unit time, P2 should have a value of 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:

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

For example:

- $Y = P1 * X *_e{}^{[-P2*K1*X]}$
- $Y = P1 * (X - P3) *_e{}^{[-P2*K1*(X-P3)]}$
- $Y = P1 * (X - P3)^{P4} *_e{}^{[-P2*K1*(X-P3)]}$

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.<br><br>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).<br><br>In the first two forms of the function P3 is assumed to be zero. |
| P4 | P4 | Growth order parameter.<br><br>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

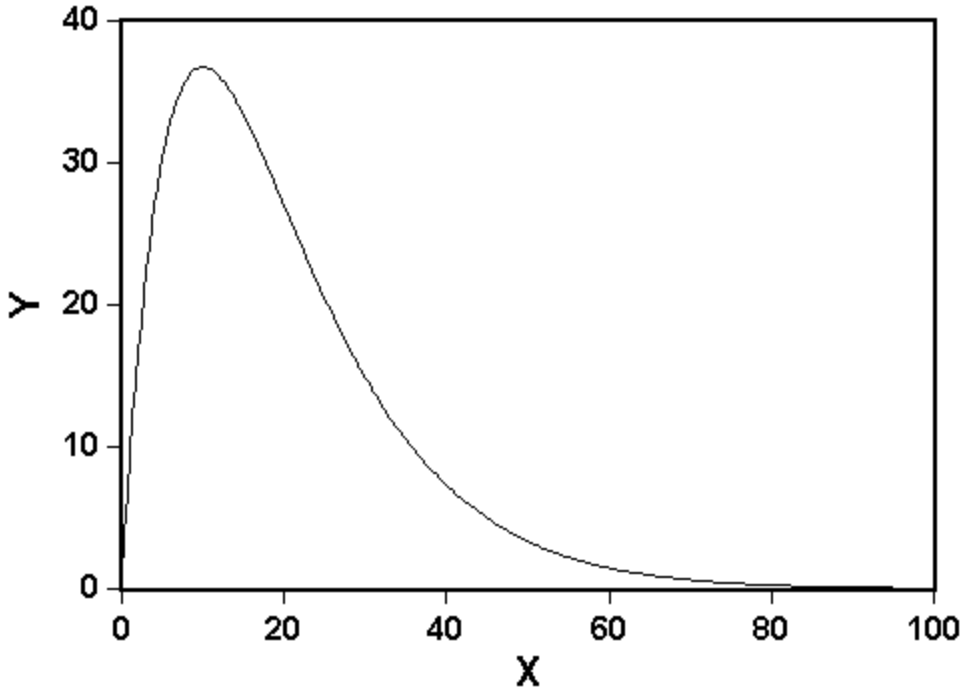
In the third form of the function, (X-P3) is assumed to be greater than zero ( > 0).

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 19

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




## *Equation*

The general form of the function is:

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

For example:

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

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.<br><br>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.<br><br>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

# 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 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 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.

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

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