

Ajustes No Lineales

El objetivo del ajuste no lineal es estimar los **valores de los parámetros** de una **función no lineal** que mejor describen los datos.

Generalmente podemos describir el proceso de ajuste de curvas no lineales de la siguiente manera:

- 1) Genere una curva de la función a partir de los valores iniciales de los parámetros.
- 2) Itere para ajustar los valores de los parámetros para acercar los puntos de datos medidos a la curva.
- 3) Deténgase cuando la distancia mínima (entre la curva y los datos) alcance algún criterio para obtener el mejor ajuste.

Ajustes No Lineales

Chi cuadrado

$$\chi^2 = \sum \frac{(O_i - E_i)^2}{E_i}$$

χ^2 lo puedo calcular siempre
(para ajustes lineales y no
lineales)

Siendo O_i los datos Observados (medidos) y E_i los datos Esperados (por el ajuste)

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Si el ajuste es bueno, se cumple la relación:

$$\chi^2 \approx \nu = N - k$$

↑
Grados de
libertad

↑
Cantidad de
parámetros

↑
Número de puntos medidos

Ajustes No Lineales

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↑
Grados de
libertad

↑
Cantidad de
parámetros

↑
Número de puntos medidos

→ Tenemos una relación
entre las variables
(vínculo)

Ajustes No Lineales

Chi cuadrado reducido

$$\chi_{\nu}^2 = \frac{\chi^2}{\nu} = \frac{\chi^2}{N-k} \left\{ \begin{array}{ll} \chi_{\nu}^2 \approx 1 & \text{✓} \\ \chi_{\nu}^2 \ll 1 & \text{✗} \rightarrow \text{Incertezas sobreestimadas} \\ \chi_{\nu}^2 \gg 1 & \text{✗} \end{array} \right.$$

Ajustes No Lineales

The screenshot displays the OriginPro 8.6 (Academic) 32-bit interface. The main window title is "OriginPro 8.6 (Academic) 32-bit - F:\Intro to Nonlinear Curve Fit Tool * - /Built-In Function/". The menu bar includes File, Edit, View, Graph, Data, Analysis, Gadgets, Tools, Format, Window, and Help. The "Analysis" menu is open, showing options like Statistics, Mathematics, Data Manipulation, Fitting, Signal Processing, and Peaks and Baseline. The "Fitting" submenu is also open, listing various fit types: Linear Fit..., Fit Linear with X Error..., Polynomial Fit..., Nonlinear Curve Fit (highlighted), Nonlinear Surface Fit..., Simulate Curve..., Simulate Surface..., Exponential Fit..., Sigmoidal Fit..., Compare Datasets..., and Compare Models... The "Nonlinear Curve Fit" option has a submenu open with "1 <Last used>" and "Open Dialog... Ctrl+Y". A yellow callout bubble points to the "Open Dialog..." option with the text "Bring up the **NLFit** dialog". In the bottom-left corner, a "Graph1" window is open, showing a plot of "Amplitude" versus "Channel". The plot features a noisy signal and a smooth Gaussian fit curve. The legend in the graph window identifies the signal as "Amplitude" and the fit as "Gauss Fit of Gauss".

Ajustes No Lineales

The screenshot displays the OriginPro 8.6 interface. The main window shows a graph titled 'Graph1' with a Gaussian curve. The data table 'Gaussian - Gaussian.dat' is visible, with columns for 'Long Name', 'Units', 'Comments', 'Sparklines', 'Channel', and 'Amplitude'. The 'NLFit ()' dialog box is open, showing the 'Function Selection' tab. A dropdown menu is open, listing various functions, with 'Gauss' highlighted. A speech bubble points to the 'Gauss' option with the text 'Select Gauss function.'.

Function Selection List:

- Allometric1
- Beta
- Boltzmann
- dHyperbl
- ExpAssoc
- ExpDec1
- ExpDec2
- ExpDec3
- ExpGrow1
- ExpGrow2
- Gauss
- GaussAmp
- Hyperbl
- Logistic
- LogNormal
- Lorentz
- Poisson
- Pulse
- Rational0
- Sine
- Voigt
- <New...>

Dialog Box Messages:

- Function is empty. Please specify it to continue.
- No Preview
- Invalid input found!
Please correct it to continue fitting.

Buttons: Fit, Done, Cancel

Play (k)

Ajustes No Lineales

OriginPro 8.6 (Academic) 32-bit - F:\Intro to Nonlinear Curve Fit Tool * - /Built-In Function/

File Edit View Graph Data Analysis Gadgets Tools Format Window Help

Default: Anal 0 B I U x² x_y x_y² α β A A'

Project Explorer (2) Quick Help Messages Log

Gaussian - Gaussian.dat

Long Name	Channel	Amplitude
Units		
Comments		
Sparklines		
1	1	
2	2	

Graph1

1

Amplitude

Channel

Amplitude

Channel

— Amplitude

— Fit Curve

NLFit (Gauss)

Dialog Theme

Settings Code Parameters Bounds

Auto Parameter Initialization

Double click cells to change operator. Right click cells for more options. Drag column header to change column orders.

NO.	Param	Meaning	Fixed	Value	Error	Dependency	Lower Conf Limits	Upper Conf Limits	Significant Digits
1	y0	offset	<input type="checkbox"/>	5.58333	--	--	--	--	System
1	xc	center	<input type="checkbox"/>	26	--	--	--	--	System
1	w	width	<input type="checkbox"/>	8.66585	--	--	--	--	System
1	A	area	<input type="checkbox"/>	976.41667	--	--	--	--	System

Fit Done Cancel

Residual Formula Sample Curve Messages Function File Hints

(1) Parameter Initialization was called.

Built-in functions have parameter initialization code, so initial parameter values are automatically assigned.



Ajustes No Lineales

The screenshot displays the OriginPro 8.6 interface. The main window shows a graph of Amplitude vs. Channel with a Gaussian fit curve. A dialog box titled "NLFit (Gauss)" is open, showing the "Parameters" tab. The parameters table is as follows:

NO.	Param	Meaning	Fixed	Value	Error	Dependency	Lower Conf Limits	Upper Conf Limits	Significant Digits
1	y0	offset	<input type="checkbox"/>	5.58333	--	--	--	--	System
1	xc	center	<input type="checkbox"/>	26	--	--	--	--	System
1	w	width	<input type="checkbox"/>	8.66585	--	--	--	--	System
1	A	area	<input type="checkbox"/>	976.41667	--	--	--	--	System

The dialog box also features a "Residual" tab, which is currently selected. It shows a plot of Regular Residual vs. A. A speech bubble points to the Residual plot with the text: "In the Residual tab, you can see the current residuals and you can judge whether the current fit results is good."

Ajustes No Lineales

The screenshot displays the OriginPro 8.6 interface. The main window shows a graph titled "Graph1" with a Gaussian fit curve overlaid on the data. The graph's y-axis is labeled "Amplitude" and the x-axis is labeled "Channel".

The "NLFit (Gauss)" dialog box is open, showing the "Parameters" tab. It contains a table of fit parameters:

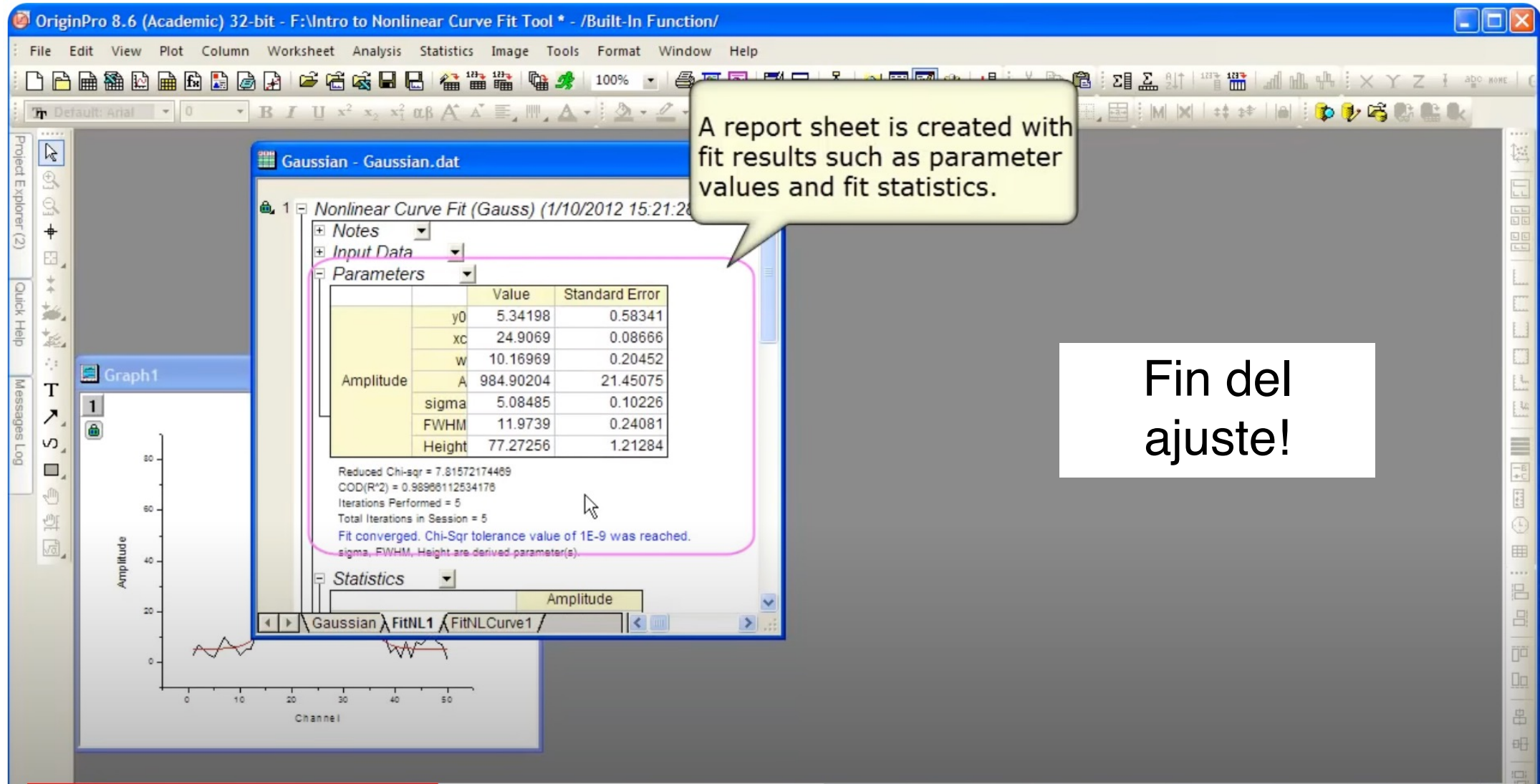
NO.	Param	Meaning	Fixed	Value	Error	Dependency	Lower Conf Limits	Upper Conf Limits	Significant Digits
1	y0	offset	<input type="checkbox"/>	5.34198	0.58341	0.54074	--	--	System
1	xc	center	<input type="checkbox"/>	24.9069	0.08666	1.07265E-11	--	--	System
1	w	width	<input type="checkbox"/>	10.16969	0.20452	0.52123	--	--	System
1	A	area	<input type="checkbox"/>	984.90204	21.45075	0.69383	--	--	System

Below the table, the "Messages" tab is selected, displaying the following text:

```
(1) Parameter Initialization was called.  
(2) -----Levenberg-Marquardt-----  
Reduced Chi-sqr = 7.81572174469  
COD(R^2) = 0.98966112534176  
Iterations Performed = 5  
Total Iterations in Session = 5  
(3) Fit converged. Chi-Sqr tolerance value of 1E-9 was reached.
```

A yellow callout box points to the "Messages" tab with the text: "Messages tab displays number of iterations, reduced chi-sqr, and R^2 values."

Ajustes No Lineales



Ajustes No Lineales

Ojo con los mínimos locales del ajuste!

Además de chequear el valor de χ^2 reducido, de R^2 y los residuos, evaluar cómo quedó el ajuste no lineal.

Si el ajuste no lineal no es bueno, estimar valores de los parámetros para poder salir del mínimo local

Ajustes No Lineales

OriginPro 8.6 (Academic) 32-bit - F:\Intro to Nonlinear Curve Fit Tool * - /Built-In Function/

File Edit View Graph Data Analysis Gadgets Tools Format Window Help

100%

Default Anal 0 B I U x² x₂ x₂ αβ A A

Project Explorer (2) Quick Help Messages Log

Graph1

1

Recalculate
Change Parameters...
Delete
Go to Source
Go to Results
Plot Input Data with Data Markers
✓ Recalculate Mode: Manual
Recalculate Mode: Auto
Recalculate Mode: None
Show Info (FitNL)
Repeat this Analysis to All Plots

Amplitude

Channel

Gaussian - Gaussian.dat

1 Nonlinear Curve Fit (Gauss) (1/10/2012 15:21:28)

Notes
Input Data
Parameters

	Value	Standard Error
Amplitude	9	0.24081
Phase	6	1.21284

Model: $y(x) = (a/b) \exp(P(x)) \exp(-x/b)$
Equation: $y(x) = (a/b) \exp(P(x)) \exp(-x/b)$
Reduced Chi-Sq: 7.21271
Std. R-Square: 0.99999

Parameter	Value	Standard Dev.
a	2.36198	0.24081
b	36.8068	0.04464
P	12.7668	0.00282
Amplitude	861.0020	21.42074
sigma	2.08185	0.10228
Phase	11.2718	0.32281
Weight	17.2728	1.21284

Value of 1E-9 was reached.
Parameter(s).

Amplitude

Bring up the **NLFit** dialog again to change the fitting option.

Opciones adicionales con Origin

Ajustes No Lineales

The screenshot displays the OriginPro 8.6 (Academic) 32-bit interface. The main window shows a graph titled "Graph 1" with "Amplitude" on the y-axis (0 to 80) and "Channel" on the x-axis (0 to 50). A black line represents the "Amplitude" data, a red line represents the "Gauss Fit", and a blue line represents the "Fit Curve". A mouse cursor is pointing at the peak of the Gaussian curve. A "Nonlinear Curve Fit (Gauss)" dialog box is open, showing the "Settings" tab. The "Function Selection" list includes "Data Selection", "Fitted Curves", "Find X/Y", "Advanced", and "Output". The "Category" is set to "Origin Basic Functions" and the "Function" is "Gauss". The "Description" is "Area version of Gaussian Function" and the "File Name(.FDF)" is "F:\sftest\NR8.6-87_90sr1_EXP\fitfunc\Gauss.fdf". The "Messages" tab at the bottom of the dialog shows the message: "(1) Parameter Initialization was called." A "Play (k)" button is visible in the bottom left corner of the graph area.

OriginPro 8.6 (Academic) 32-bit - F:\Intro to Nonlinear Curve Fit Tool * - /Built-In Function/

File Edit View Graph Data Analysis Gadgets Tools Format Window Help

Default Anal 0 B I U x² x₂ x₂ α β A A

Project Explorer (2) Quick Help Messages Log

Gaussian - Gaussian.dat

1 Nonlinear Curve Fit (Gauss)

Notes

Input Data

Parameters

Graph 1

1

Amplitude

Channel

Amplitude

Gauss Fit

Fit Curve

Model: $y = y_0 + (x - xc) \cdot \exp(-\frac{(x - xc)^2}{2 \cdot \sigma^2})$

Parameter	Value	Standard Error
xc	23.37195	0.24
yc	24.90949	0.24
sigma	10.71699	0.22
sigma	861.8000	19.12
Amplitude	2.58185	0.12
Position	11.9759	0.24
Width	11.27054	1.2

Dialog Theme

Settings Code Parameters Bounds

Function Selection

Data Selection

Fitted Curves

Find X/Y

Advanced

Output

Category: Origin Basic Functions

Function: Gauss

Description: Area version of Gaussian Function

File Name(.FDF): F:\sftest\NR8.6-87_90sr1_EXP\fitfunc\Gauss.fdf

Fit Done Cancel

Residual Formula Sample Curve Messages Function File Hints

(1) Parameter Initialization was called.

Play (k)

Ajustes No Lineales

The screenshot displays the OriginPro 8.6 (Academic) 32-bit interface. The main window shows a graph titled "Graph 1" with "Amplitude" on the y-axis and "Channel" on the x-axis. A signal is plotted with a red Gaussian fit curve. A "Gaussian - Gaussian.dat" window is open, showing the "Parameters" tab with the following data:

NO.	Param	Meaning	Fixed	Value	Significant Digits
1	y0	offset	<input type="checkbox"/>	5.34198	System
1	xc	center	<input type="checkbox"/>	24.9069	System
1	w	width	<input type="checkbox"/>	10.16969	System
1	A	area	<input type="checkbox"/>	984.90204	System

The "NLFit (Gauss)" dialog box is open, showing the "Parameters" tab. A yellow callout bubble points to the "xc" parameter value, containing the text: "Fix the value of center to 25." The dialog also includes a "Messages" tab with the following text:

(1) Parameter Initialization was called.

At the bottom left of the graph area, there is a "Play (k)" button.

Ajustes No Lineales

OriginPro 8.6 (Academic) 32-bit - F:\Intro to Nonlinear Curve Fit Tool * - /Built-In Function/

File Edit View Plot Column Worksheet Analysis Statistics Image Tools Format Window Help

Default: Arial 0 B I U x² x₂ x₂ α β A A

Project Explorer (2) Quick Help Messages Log

Graph1

Amplitude

Channel

Play (k)

Gaussian - Gaussian.dat

1 Nonlinear Curve Fit (Gauss) (1/10/2012 15:22:18)

Notes

Input Data

Parameters

	Value	Standard Error
y0	5.34629	0.58432
xc	25	0
w	10.16855	0.2048
Amplitude A	984.68626	21.48327
sigma	5.08427	0.10243
FWHM	11.97255	0.24121
Height	77.26433	1.21488

Reduced Chi-sqr = 7.84134711285
COD(R²) = 0.98940173228649
Iterations Performed = 2
Total Iterations in Session = 2
Fit converged. Chi-Sqr tolerance value of 1E-9 was reached.
Some parameter values were fixed.
sigma, FWHM, Height are derived parameter(s).

Statistics

Gaussian FitNL1 FitNLCurve1

Error value is zero because parameter value was fixed.