

Chapter 380

Sum of Functions Models

Introduction

This program fits models that are the ratio of two linear expressions. The general form of a model is:

$$g(Y) = \frac{A0 + A1f_1(X) + A2f_2(X) + A3f_3(X) + A4f_4(X) + A5f_5(X)}{1 + B1h_1(X) + B2h_2(X) + B3h_3(X) + B4h_4(X) + B5h_5(X)} + e$$

where $f_i(X)$, $g(Y)$, and $h_i(X)$ are standard functions such as $\text{SIN}(X)$, $\text{LN}(X+1)$, $\text{SQRT}(X/2)$, etc. The $A0$, $A1$, ..., $B5$ are constants (parameters) to be estimated from the data.

These models approximate many different curves. They offer a much wider variety of curves than the usual polynomial models.

Since these are approximating curves and have no physical interpretation, care must be taken outside the range of the data. You must study the resulting model graphically to determine that the model behaves properly between data points.

Starting Values

Starting values are determined by the program from the data. You do not have to supply starting values.

Assumptions and Limitations

Usually, nonlinear regression is used to estimate the parameters in a nonlinear model without performing hypothesis tests. In this case, the usual assumption about the normality of the residuals is not needed. Instead, the main assumption needed is that the data may be well represented by the model.

Data Structure

The data are entered in two variables: one dependent variable and one independent variable.

Missing Values

Rows with missing values in the variables being analyzed are ignored in the calculations. When only the value of the dependent variable is missing, predicted values are generated.

Model – Numerator and Denominator Terms

The user may specify up to five terms for use as the numerator and/or denominator of the model. You do not have to have a denominator.

Function

There are eighteen possible transformations.

$f(z) = 1/(z^2)$	$f(z) = 1/z$	$f(z) = 1/SQRT(z)$
$f(z) = LN(z)$	$f(z) = SQRT(z)$	$f(z) = z$ (<i>none</i>)
$f(z) = z^2=z*z$	$f(z) = z^3$	$f(z) = z^4$
$f(z) = z^5$	$f(z) = EXP(z)$	$f(z) = EXP(-z)$
$f(z) = SIN(z)$	$f(z) = COS(z)$	$f(z) = TAN(z)$
$f(z) = SINH(z)$	$f(z) = COSH(z)$	$f(z) = TANH(z)$

where

$z = MX+A$; M and A are constants that are supplied in the two options below.

Example 1 – Fitting a Sum of Functions Model

This section presents an example of how to fit a sum of functions model. In this example, we will fit the model

$$Y = A_0 + A_1/(X+0.5) + \sin(X/2) + A_3 \tanh(X)$$

to the variables Y and X of the FnReg1 database.

Setup

To run this example, complete the following steps:

1 Open the FnReg1 example dataset

- From the File menu of the NCSS Data window, select **Open Example Data**.
- Select **FnReg1** and click **OK**.

2 Specify the Sum of Functions Models procedure options

- Find and open the **Sum of Functions Models** procedure using the menus or the Procedure Navigator.
- The settings for this example are listed below and are stored in the **Example 1** settings template. To load this template, click **Open Example Template** in the Help Center or File menu.

<u>Option</u>	<u>Value</u>
Variables Tab	
Y (Dependent)	Y
X (Independent)	X
Function 1	1/z
Add (A)	0.5
Function 2	SIN(z)
Multiply (M)	0.5
Function 3	TANH(z)
Reports Tab	
Residual Report	Checked
All Other Reports and Plots	Checked

3 Run the procedure

- Click the **Run** button to perform the calculations and generate the output.

Minimization Phase Section

Minimization Phase Section

Itn	Error Sum					
No.	Lambda	Lambda	A0	A1	A2	A3
0	5.915745	4E-05	2.070158	4.885924	1.059697	7.084624

Convergence criterion met.

This report displays the error (residual) sum of squares, lambda, and parameter estimates for each iteration. It allows you to observe the algorithm's progress. Since no denominator terms were selected, the model was solved on the first iteration using standard multiple linear regression.

Model Estimation Section

Model Estimation Section				
Parameter Name	Parameter Estimate	Asymptotic Standard Error	Lower 95% C.L.	Upper 95% C.L.
A0	2.070158	1.075332	-0.06435942	4.204676
A1	4.885924	0.5628729	3.768631	6.003218
A2	1.059697	0.06202012	0.9365882	1.182806
A3	7.084624	0.9798195	5.139698	9.029551
Dependent	Y			
Independent	X			
Model	Y=A0+A1*(1/(X+0.5))+A2*(SIN((0.5*X)))+A3*(TANH(X))			
R-Squared	0.956784			
Iterations	0			
Estimated Model				
(2.070158+(4.885924)*1/(X+0.5)+(1.059697)*SIN((0.5*X))+(7.084624)*TANH(X))				

Parameter Name

The name of the parameter whose results are shown on this line.

Parameter Estimate

The estimated value of this parameter.

Asymptotic Standard Error

An estimate of the standard error of the parameter based on asymptotic (large sample) results.

Lower 95% C.L.

The lower value of a 95% confidence limit for this parameter. This is a large sample (at least 25 observations for each parameter) confidence limit.

Upper 95% C.L.

The upper value of a 95% confidence limit for this parameter. This is a large sample (at least 25 observations for each parameter) confidence limit.

Model

The model that was estimated. Use this to double check that the model estimated was what you wanted. Note that the “/(1)” at the end emphasizes that there was no denominator specified.

R-Squared

There is no direct R-Squared defined for nonlinear regression. This is a pseudo R-Squared constructed to approximate the usual R-Squared value used in multiple regression. We use the following generalization of the usual R-Squared formula:

$$R\text{-Squared} = (ModelSS - MeanSS)/(TotalSS - MeanSS)$$

where *MeanSS* is the sum of squares due to the mean, *ModelSS* is the sum of squares due to the model, and *TotalSS* is the total (uncorrected) sum of squares of Y (the dependent variable).

This version of R-Squared tells you how well the model performs after removing the influence of the mean of Y. Since many nonlinear models do not explicitly include a parameter for the mean of Y, this R-Squared may be negative (in which case we set it to zero) or difficult to interpret. However, if you think of it as a direct extension of the R-Squared that you use in multiple regression, it will serve well for comparative purposes.

Iterations

The number of iterations that were completed before the nonlinear algorithm terminated. If the number of iterations is equal to the Maximum Iterations that you set, the algorithm did not converge, but was aborted.

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Estimated Model

The model that was estimated with the parameters replaced with their estimated values. This expression may be copied and pasted as a variable transformation in the spreadsheet. This will allow you to predict for additional values of X.

Analysis of Variance Table

Analysis of Variance Table			
Source	DF	Sum of Squares	Mean Square
Mean	1	10559.48	10559.48
Model	4	10690.45	10694.89
Model (Adjusted)	3	130.9726	43.65752
Error	96	5.915745	0.06162234
Total (Adjusted)	99	136.8883	
Total	100	10696.37	

Source

The labels of the various sources of variation.

DF

The degrees of freedom.

Sum of Squares

The sum of squares associated with this term. Note that these sums of squares are based on Y, the dependent variable. Individual terms are defined as follows:

Mean	The sum of squares associated with the mean of Y. This may or may not be a part of the model. It is presented since it is the amount used to adjust the other sums of squares.
Model	The sum of squares associated with the model.
Model (Adjusted)	The model sum of squares minus the mean sum of squares.
Error	The sum of the squared residuals. This is often called the sum of squares error or just "SSE."
Total	The sum of the squared Y values.
Total (Adjusted)	The sum of the squared Y values minus the mean sum of squares.

Mean Square

The sum of squares divided by the degrees of freedom. The Mean Square for Error is an estimate of the underlying variation in the data.

Asymptotic Correlation Matrix of Parameters

Asymptotic Correlation Matrix of Parameters				
	A0	A1	A2	A3
A0	1.000000	-0.972405	0.786167	-0.999209
A1	-0.972405	1.000000	-0.831952	0.964719
A2	0.786167	-0.831952	1.000000	-0.779440
A3	-0.999209	0.964719	-0.779440	1.000000

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This report displays the asymptotic correlations of the parameter estimates. When these correlations are high (absolute value greater than 0.95), the precision of the parameter estimates is suspect.

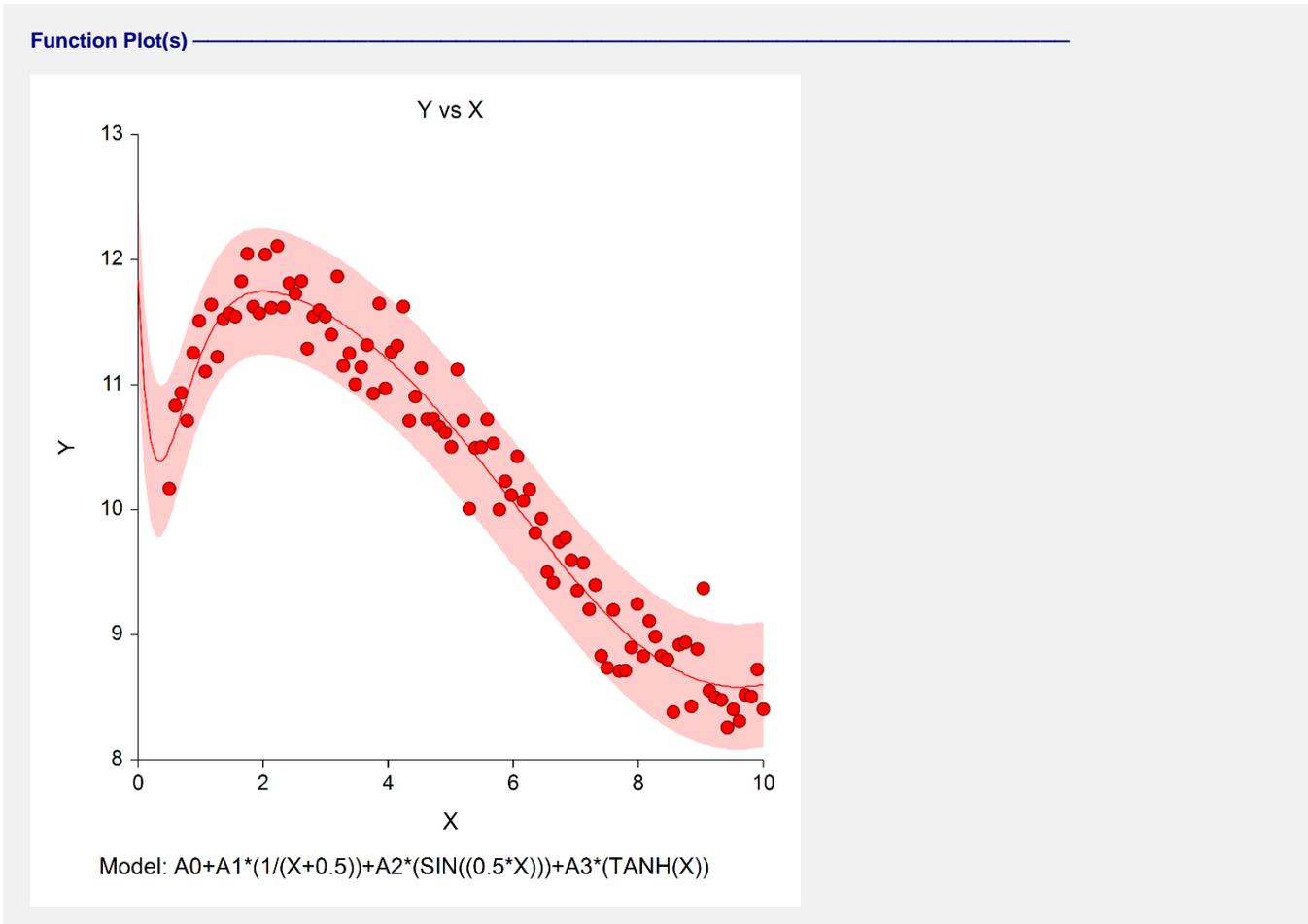
Predicted Values and Residuals Section

Predicted Values and Residuals Section

Row No.	X	Y	Predicted Value	Lower 95.0% Value	Upper 95.0% Value	Residual
1	0.5	10.16989	10.49218	9.92255	11.06181	-0.3222909
2	0.5959596	10.83415	10.62378	10.07584	11.17172	0.2103729
3	0.6919192	10.93412	10.77391	10.24289	11.30493	0.1602088
4	0.7878788	10.71519	10.92673	10.40745	11.44602	-0.2115456
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The section shows the values of the residuals and predicted values. If you have observations in which the independent variable is given, but the dependent (Y) variable was left blank, a predicted value and prediction limits will be generated and displayed in this report.

Function Plot(s)

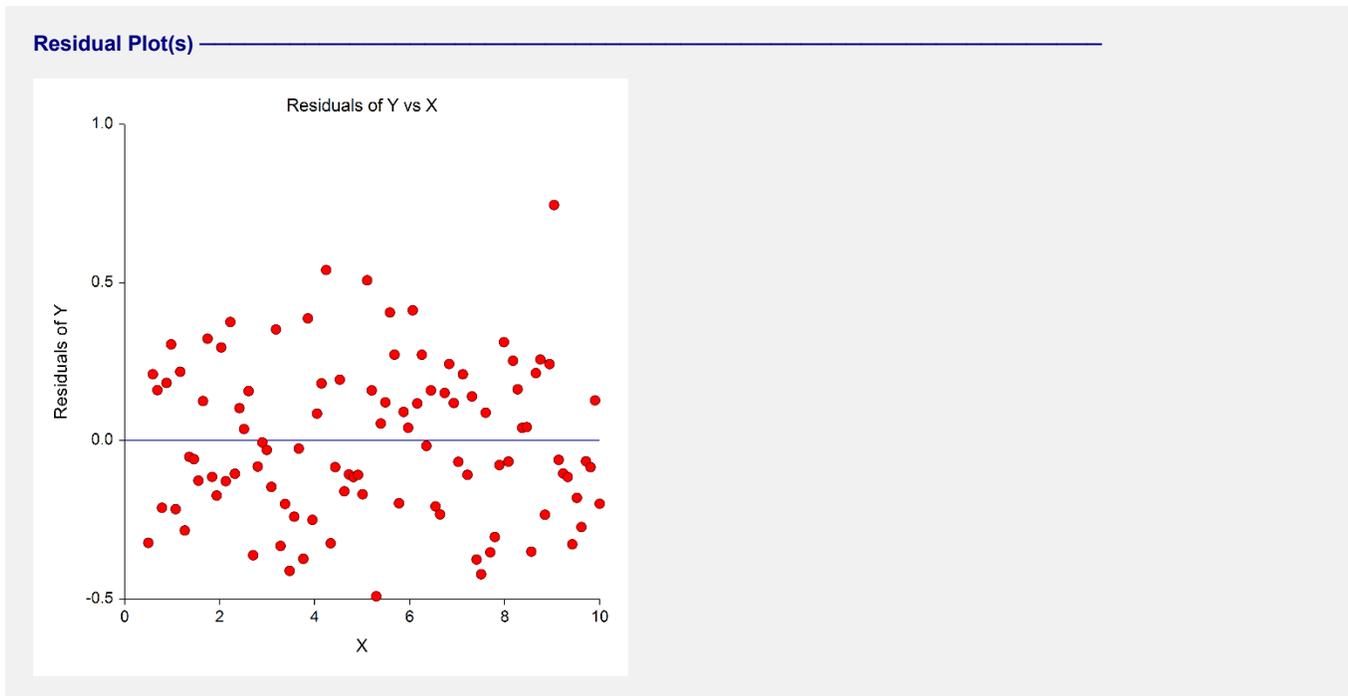


This plot displays the data along with the estimated function and prediction limits. It is useful in deciding if the fit is adequate and the prediction limits are appropriate.

Sum of Functions Models

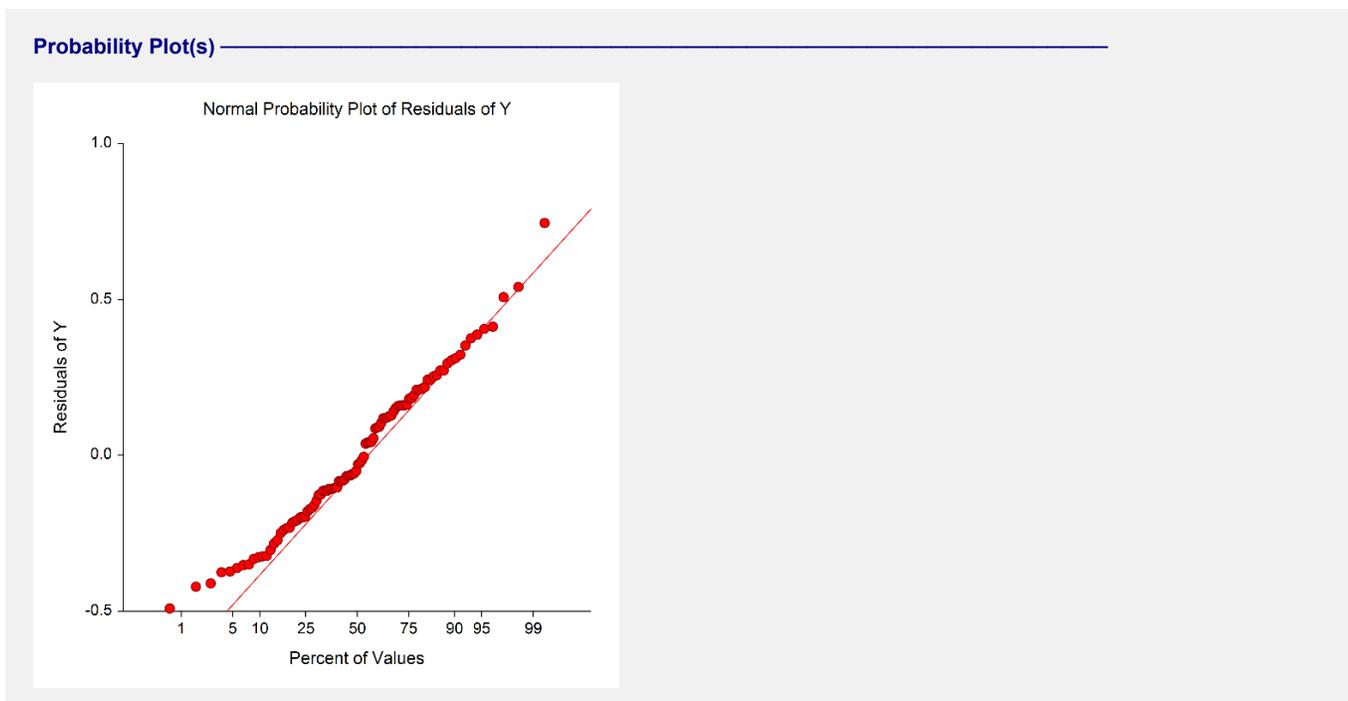
In poorly fit models, we have found that it is often necessary to disable the prediction limits so that the data will show up. In these cases, the prediction limits may be so wide that the scale of the plot does not allow the data values to be separated.

Residual Plot(s)



This is a scatter plot of the residuals versus the independent variable, X. The preferred pattern is a rectangular shape or point cloud. Any nonrandom pattern may require a redefining of the model.

Probability Plot(s)



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If the residuals are normally distributed, the data points of the normal probability plot will fall along a straight line. Major deviations from this ideal picture reflect departures from normality. Stragglers at either end of the normal probability plot indicate outliers, curvature at both ends of the plot indicates long or short distributional tails, convex or concave curvature indicates a lack

of symmetry, and gaps or plateaus or segmentation in the normal probability plot may require a closer examination of the data or model. We do not recommend that you use this diagnostic with small sample sizes.

Predicting for New Values

You can use your model to predict Y for new values of X. Here's how. Add new rows to the bottom of your database containing the values of the independent variable that you want to create predictions for. Leave the dependent variable blank. When the program analyzes your data, it will skip these rows during the estimation phase, but it will generate predicted values for all rows, regardless of whether the Y variable is missing or not.