

Chapter 330

Response Surface Regression

Introduction

This *Response Surface Analysis* (RSA) program fits a polynomial regression model with cross-product terms of variables that may be raised up to the third power. It calculates the minimum or maximum of the surface. The program also has a variable selection feature that helps you find the most parsimonious hierarchical model. NCSS automatically scans the data for duplicates so that a lack-of-fit test may be calculated using pure error.

One of the main goals of RSA is to find a polynomial approximation of the true nonlinear model, similar to the Taylor's series expansion used in calculus. Hence, you are searching for an approximation that works well in a specified region. As the region is reduced, the number of terms may also be reduced. In a very small region, a linear (first-order) approximation may be adequate. A larger region may require a quadratic (second-order) approximation.

Hierarchical Models

In the following discussion, the X's are independent variables with at least three distinct values (up to six X's may be specified). Y is the dependent variable. Z is a covariate (note that covariates do not have to have three or more levels). The β 's are the regression coefficients or beta weights.

A polynomial model is one in which the X's occur as multiples of each other. Examples of polynomial models are:

$$Y_j = \beta_0 + \beta_1 X_{1j} + \varepsilon_j$$

$$Y_j = \beta_0 + \beta_1 X_{1j} + \beta_2 X_{2j} + \beta_3 X_{1j} X_{2j} + \varepsilon_j$$

$$Y_j = \beta_0 + \beta_1 X_{1j} + \beta_2 X_{2j}^2 + \beta_3 X_{1j}^2 X_{2j}^3 + \varepsilon_j$$

A hierarchical model obeys the following rule: all lower-order terms that can be constructed by reducing the exponents of the variables in a term are also in the model. For example, if the term $X_1 X_2^2$ is in the model, so are X_1 , X_2 , $X_1 X_2$, and X_2^2 . Notice that each of these terms can be created by decreasing the exponents of the two variables that form the original term (noting that $X_0 = 1$). Note that the first two models are hierarchical, but the third is not.

Hierarchical models enjoy several useful properties, including stability, the ability to change the scale (coding) of a variable, and a general relationship with ANOVA modeling. However, they usually require the fitting of more parameters than nonhierarchical models. This NCSS procedure fits only hierarchical models. If nonhierarchical models are desired, they can be fit using the Multiple Regression module.

Model Selection

There are several strategies to variable selection and model building in regression analysis: forward selection, backward elimination, stepwise, all possible regressions, and more. However, none of these methods guarantee hierarchical models. We need a method that does. This NCSS program adopts a strategy that has been used for quite a while in dealing with hierarchical models. The strategy may be outlined as follows:

1. Begin with the most complicated model desired. NCSS allows terms of the form $X_i^i X_j^j$, where i and j are each less than or equal to three.
2. Search through all terms, marking those that are not necessary to maintain the hierarchical constraint on the model. This group of terms is available for removal.
3. Check each of the available terms to determine how much R-Squared is decreased if they are removed.
4. Remove the term that decreases R-Squared the least. Return to step 2. Note that this variable is never reconsidered for inclusion in the model.
5. If no available term can be identified that reduces R-Squared by an amount that is less than the specified cutoff value, the model selection procedure is terminated.

Assumptions and Limitations

The same assumptions and qualifications apply here as applied to multiple regression. We refer you to the Assumptions section in the Multiple Regression chapter for a discussion of these assumptions. We will here mention a couple of restrictions necessary for this algorithm to work.

Number of Observations

The number of observations must be at least one greater than the number of terms (including all cross products). A popular rule-of-thumb when using any variable selection procedure is that you have at least five observations for each term.

Unique Data Values

Since various powers of the variables are included, the structure of your data must allow for these powers to be fit. This means that if the maximum exponent on a variable is k , the number of unique values in that variable must be at least $k+1$. For example, suppose a variable consisted of two values: -1 and 1. You could not fit a model that included more than a linear ($k=1$) term in this variable. Again, suppose your data consisted of three values: -1,0,1. The maximum exponent that could be used with this variable is 2.

Data Structure

The data are entered in two or more columns. An example of data appropriate for this procedure is shown in the following table and is found in the Odor dataset. This dataset relates a measurement of odor to three variables in a chemical process. Fifteen rows of data were obtained. The values of the three independent variables have been recoded so that they are -1, 0, and 1. A sixteenth row has been added. Notice that it does not contain a value in the *Odor* column. A predicted value will be generated for this row, but its values will not be used in the estimation process.

We suggest that you open this dataset now so that you can follow along with the example.

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Odor dataset

Odor	Temp	Ratio	Height
66	-1	-1	0
58	-1	0	-1
65	0	-1	-1
-31	0	0	0
39	1	-1	0
17	1	0	-1
7	0	1	-1
-35	0	0	0
43	-1	1	0
-5	-1	0	1
43	0	-1	1
-26	0	0	0
49	1	1	0
-40	1	0	1
-22	0	1	1
	1	1	0

Missing Values

Rows with missing values in the variables being analyzed are ignored. If data are present for all but the dependent variable, a predicted value is generated for this row.

Procedure Options

This section describes the options available in this procedure.

Variables Tab

This panel specifies the variables used in the analysis.

Dependent Variable

Dependent Variable (Y☺)

Specifies the dependent (Y) variable.

Plot Minimum

This option lets you set a minimum for the depth (dependent variable) axis. If left blank, it is determined from the data.

Plot Maximum

This option lets you set a maximum for the depth (dependent variable) axis. If left blank, it is determined from the data.

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Factor Variables

Factor Variable (A - F)

Specifies the variables to be used as independent variables. Each of these variables must be categorical—have only a few unique values. Think of A as X_1 , B as X_2 , etc. The terms of the hierarchical model will be generated from these variables. Note that each variable must have enough unique values to fit the highest exponent required of it in the model:

<u>Number of Unique Values</u>	<u>Largest Exponent Possible</u>
2	1 (linear)
3	2 (quadratic)
4	3 (cubic)

Constant

This option lets you specify a constant value to be used for this variable when it is not one of the pair of factors being displayed on the grid plot. If you leave this option blank, the factor average will be used.

Minimum

This option lets you set a minimum for the axis related to this factor. If left blank, it is determined from the data.

Maximum

This option lets you set a maximum for the axis related to this factor. If left blank, it is determined from the data.

Decimals

This specifies the number of decimal places displayed in the reference numbers on axis showing this factor.

Covariates

Covariate Variables

These are other independent variables included in the regression model, but their powers and cross-products will not be generated. They are not part of the “response surface.”

Model Tab

These boxes define the hierarchical model in a shorthand notation.

Model Specification – Order

Order (A - F)

These boxes define the maximum exponent for each factor. Values from one to three are allowed. All terms of order less than or equal to this value are included in the model. For example, a ‘2’ implies that X and X^2 are included.

Model Specification – Maximum Orders of Two-Way Terms

Maximum Orders of Two-Way Terms (AB - EF)

These boxes define the maximum exponent for each factor in the cross-product term of the corresponding variables. For example, “AC” represents the product of factors A and C.

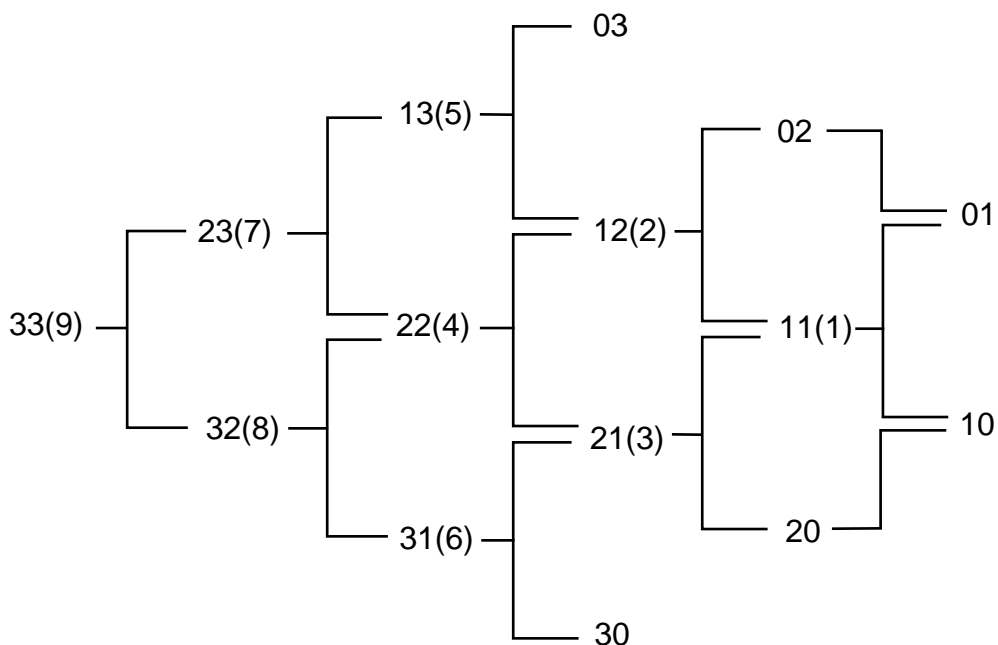
All subset terms (children) are also included in the model, so that the hierarchical nature of the model is maintained.

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A code is used to specify the maximum exponents of each term. Up to three of these may be needed to specify the desired hierarchical model. The following table relates each coded value to the terms that it generates. This table will be generated for the *AB* term. The pattern extends in an obvious manner to the other cross-products. Note that a “10” is used to represent A, a “01” represents B, a “20” represents A², and so on.

<u>Code</u>	<u>Term(s)</u>	<u>Cross Product Terms Actually Included</u>
1	11	AB
2	12	AB, AB2
3	21	AB, A2B
23	12,21	AB, AB2, A2B
4	22	AB, A2B, AB2, A2B2
5	13	AB, AB2, AB3
35	21,13	AB, A2B, AB2, AB3
45	22,13	AB, A2B, AB2, A2B2, AB3
6	31	AB, A2B, A3B
26	12,31	AB, AB2, A2B, A3B
46	22,31	AB, AB2, A2B, A2B2, A3B
56	13,31	AB, AB2, A2B, AB3, A3B
456	22,13,31	AB, AB2, A2B, AB3, A3B, A2B2
7	23	AB, A2B, AB2, A2B2, AB3, A2B3
67	31,23	AB, A2B, AB2, A2B2, AB3, A3B, A2B3
8	32	AB, AB2, A2B, A2B2, A3B, A3B2
58	13,32	AB, AB2, A2B, A2B2, AB3, A3B, A3B2
78	23,32	AB, AB2, A2B, A2B2, AB3, A3B, A2B3, A3B2
9	33	AB, AB2, A2B, A2B2, A3B, A3B2, AB3, A2B3, A3A3

The following tree diagram shows the hierarchical structure of this system. Each term generates all terms to the right of it. These terms are called *children*. A term that is a child of one term is not specified with that term. For example, terms 13, 22, and 31 could be selected together. However, the terms 23 and 21 could not be entered together since 21 is a child of 23 and will automatically be included when 23 is specified. Note the cross-product terms include their codes in parentheses. Also note that terms like 03 and 20 are specified in the One-Way Terms section.



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The actual specification of the term is accomplished by selecting one or more codes from a list of possible models. For example, you might select “58.” This model represents the 13 and the 32 terms plus all their children.

The usual quadratic model is specified by selecting 2’s for the Order terms and 1’s for the Two-Way terms.

Model Selection

Conduct Model Selection

Specifies whether to search (checked) for the most parsimonious hierarchical model or simply fit the one that is specified (unchecked).

Minimum R-Squared Kept

Sets the minimum amount that an available term must add to the overall R-Squared to avoid being removed from the model. Note that this is the amount that the R-Squared is decreased if only this term is removed, leaving all other terms in the model.

Optimization Tab

These options control the Hooke and Jeeves optimization routine as described in Nash (1987).

Optimization Options

Optimization Goal

Specifies whether a minimum or maximum is sought.

Maximum Evaluations

Specifies the maximum number of function evaluations before the routine is aborted.

Set Linear Factors to Mean Values

Specifies whether linear-only variables should be set to their mean values or left to vary. Usually, you would set these to their mean values since a straight line has no minimum or maximum.

Set Cubic Factors to Mean Values

Specifies whether cubic variables should be set to their mean values or left to vary. Usually, you would set these to their mean values since a cubic function has no minimum or maximum.

Reports Tab

The following options control which reports are displayed.

Select Reports

Descriptive Statistics ... Residuals Reports

Specifies whether to output the various reports.

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Report Options

Precision

Specify the precision of numbers in the report. Single precision will display seven-place accuracy, while double precision will display thirteen-place accuracy.

Variable Names

This option lets you select whether to display variable names, variable labels, or both.

Report Options – Decimal Places

Response and Beta Decimals

Specify the number of digits after the decimal point to display on the output of values of this type. Note that this option in no way influences the accuracy with which the calculations are done.

Plots Tab

The options on this panel control the inclusion and the appearance of the plots.

Select Plots

Probability Plot and Contour Plots

Specifies whether to output these plots. Click the plot format button to change the plot settings.

Storage Tab

Various statistics calculated for each row may be stored on the current database for further analysis. This group of options lets you designate which statistics (if any) should be stored and which variables should receive these statistics. The selected statistics are automatically stored to the current database while the program is running.

The variables you specify must already have been defined on the current database. Remember that existing data will be replaced. Following is a description of the statistics that can be stored.

Data Storage Variables

Predicted Values

The predicted (\hat{Y}) values.

Residuals

The residuals ($Y - \hat{Y}$).

Expanded Factors

If you are going to analyze your data further using another regression module, you will need to generate the squares, cubes, and cross-product terms using Variable Transformations. This option lets you store these variables directly on the database. New variables containing all $X_i^I X_j^J$ for all values of $i, I, j,$ and J in the current model will be created.

Example 1 – Response Surface Analysis

This section presents an example of how to run a response surface analysis of the data contained in the Odor dataset.

You may follow along here by making the appropriate entries or load the completed template **Example 1** by clicking on Open Example Template from the File menu of the Response Surface Regression window.

1 Open the Odor dataset.

- From the File menu of the NCSS Data window, select **Open Example Data**.
- Click on the file **Odor.NCSS**.
- Click **Open**.

2 Open the Response Surface Regression window.

- Using the Analysis menu or the Procedure Navigator, find and select the **Response Surface Regression** procedure.
- On the menus, select **File**, then **New Template**. This will fill the procedure with the default template.

3 Specify the variables.

- On the Response Surface Regression window, select the **Variables tab**.
- Double-click in the **Dependent Variable** text box. This will bring up the variable selection window.
- Select **Odor** from the list of variables and then click **Ok**. “Odor” will appear in the Dependent Variable box.
- Double-click in the **Factor Variable - A** text box. This will bring up the variable selection window.
- Select **Temp** from the list of variables and then click **Ok**.
- Double-click in the **Factor Variable - B** text box. This will bring up the variable selection window.
- Select **Ratio** from the list of variables and then click **Ok**.
- Double-click in the **Factor Variable - C** text box. This will bring up the variable selection window.
- Select **Height** from the list of variables and then click **Ok**.
- On the plots tab, increase the Number of X Slices and Number of Y Slices to 50 or 100 for a higher resolution contour plot.

4 Run the procedure.

- From the Run menu, select **Run Procedure**. Alternatively, just click the green Run button.

Descriptive Statistics Section

Descriptive Statistics Section

Variable	Count	Mean	Minimum	Maximum
Temp	15	0	-1	1
Ratio	15	0	-1	1
Height	15	0	-1	1
Odor	15	15.2	-40	66

This report provides the count, mean, minimum, and maximum of each of the variables in the analysis. It allows you to determine if the data fall within reasonable limits.

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Hierarchical Model Summary Section

Hierarchical Model Summary Section

Number of Terms Removed	0
Number of Terms Remaining	9
R-Squared Cutoff Value	0.010000
R-Squared of Final Model	0.881989

Coded Hierarchical Model

	A	B	C
A Temp	2	1(11)	1(11)
B Ratio		2	1(11)
C Height			2

Notes:

For off-diagonal entries:

1= u_1w_1 , 2= u_1w_2 , 3= u_2w_1 , 4= u_2w_2 , 5= u_1w_3 , 6= u_3w_1 , 7= u_2w_3 , 8= u_3w_2 , 9= u_3w_3 .

For diagonal entries:

1= u_1 , 2= u_2 , 3= u_3 .

Where $u_1=u$, $u_2=u^2=u*u$, and $u_3=u^3=u*u*u$.

This report shows the hierarchical model that was specified. It also shows the final R-Squared value as well as the R-Squared cutoff that was used. It is mainly used to document the model used.

The specified model is determined by considering all nonzero entries. The *Notes* section at the bottom shows how the model is determined. For example, the first line is nonzero for the *terms* AA, AB, and AC. These codes represent the terms: Temp², (Temp)(Ratio), and (Temp)(Height). All child terms necessary to make this a hierarchical model are also generated.

Sequential ANOVA Section

Sequential ANOVA Section

Source	DF	Sequential Sum-Squares	Mean Square	F-Ratio	Prob Level	Incremental R-Squared
Regression	9	18881.98	2097.998	4.15	0.065691	0.881989
Linear	3	7143.25	2381.083	4.71	0.064071	0.333666
Quadratic	3	11445.23	3815.078	7.55	0.026426	0.534614
Lin x Lin	3	293.5	97.83334	0.19	0.896470	0.013710
Total Error	5	2526.417	505.2833			0.118011
Lack of Fit	3	2485.75	828.5833	40.75	0.024047	0.116111
Pure Error	2	40.66667	20.33333			0.001900

Sequential ANOVA Section Using Pure Error

Source	DF	Sequential Sum-Squares	Mean Square	F-Ratio	Prob Level	Incremental R-Squared
Regression	9	18881.98	2097.998	103.18	0.009635	0.881989
Linear	3	7143.25	2381.083	117.10	0.008479	0.333666
Quadratic	3	11445.23	3815.078	187.63	0.005306	0.534614
Lin x Lin	3	293.5	97.83334	4.81	0.176872	0.013710
Total Error	5	2526.417	505.2833			0.118011
Lack of Fit	3	2485.75	828.5833	40.75	0.024047	0.116111
Pure Error	2	40.66667	20.33333			0.001900

This display actually shows two reports. The top is the regular Sequential ANOVA Section defined below. Note that the denominator of the F-Ratios is the Total Error Mean Square. The bottom report is identical to the top, except that the denominator of the F-Ratios is now the Pure Error Mean Square.

This report is designed with two main goals:

1. Determine the sequential influence of the various power and cross-product terms.
2. Test for model lack of fit if repeated observations are available.

Response Surface Regression

Source

The group of independent variables being tested.

Regression	Total of all terms in the model.
Linear	The total for X_i terms.
Quadratic	The total for X_i^2 terms.
Cubic	The total for X_i^3 terms.
Lin x Lin	The total for $X_i X_j$ terms.
Lin x Quad	The total for $X_i X_j^2$ terms.
Quad x Quad	The total for $X_i^2 X_j^2$ terms.
Lin x Cubic	The total for $X_i X_j^3$ terms.
Quad x Cubic	The total for $X_i^2 X_j^3$ terms.
Cubic x Cubic	The total for $X_i^3 X_j^3$ terms.

DF

The degrees of freedom associated with the group of terms.

Sequential Sum-Squares

The regression sum of squares added sequentially by each group of terms. Each group of terms adds this amount of sum of squares after accounting for the terms above it in the report.

Mean Square

The sum of squares divided by the degrees of freedom.

F-Ratio

The F-value formed by dividing the Mean Square by the Total Error Mean Square. Note that these tests are sequential in nature and should be considered from the bottom up. Note that in the second report, the Total Error Mean Square is replaced by the Pure Error Mean Square as the denominator of the F-ratio.

In the above example, the Lin x Lin F-ratio tests whether the linear-by-linear terms are significant in the regression model after considering the linear and quadratic terms. The Quadratic F-ratio tests whether the quadratic terms add significantly to a model consisting of the linear terms (ignoring the linear-by-linear terms).

In terms of the ODOR data, the tests are interpreted as follows:

<u>Group</u>	<u>Terms</u>	<u>Hypothesis Tested</u>
Lin x Lin	Temp x Ratio Temp x Height Ratio x Height	All coefficients of these variables are zero.
Quadratic	Temp x Temp Ratio x Ratio Height x Height	All coefficients of these variables are zero, ignoring the influence of the cross-product terms.
Linear	Temp Ratio Height	All coefficients of these variables are zero, ignoring the influence of the cross-product and quadratic terms

Prob Level

This is the right-tail probability or significance level of this test. Reject the hypothesis that the influence of the terms is zero when this value is less than a predetermined value of alpha, say 0.05.

Incremental R-Squared

The first line displays the total R-Squared for the complete model. The other lines display the amount of R-Squared that is added by each group of terms. Hence, the total of the rest of the lines equals the first.

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Lack of Fit and Pure Error

These lines are only displayed if you have repeated observations from which the variability between identical observations may be estimated. The lack of fit tests the adequacy of the specified model. A significant F-test implies that a higher-order polynomial (such as cubic) or a different functional form would fit the data better.

If pure error is available, the F-tests are recalculated using the Pure Error Mean Square as the denominator rather than the Total Error Mean Square.

ANOVA Section

ANOVA Section						
Factor	DF	Last Sum-Squares	Mean Square	F-Ratio	Prob Level	Term R-Squared
Temp	4	5258.016	1314.504	2.60	0.161334	0.245605
Ratio	4	11044.6	2761.151	5.46	0.045377	0.515900
Height	4	3813.016	953.254	1.89	0.251025	0.178108
Total Error	5	2526.417	505.2833			0.118011
Lack of Fit	3	2485.75	828.5833	40.75	0.024047	0.116111
Pure Error	2	40.66667	20.33333			0.001900

ANOVA Section Using Pure Error						
Factor	DF	Last Sum-Squares	Mean Square	F-Ratio	Prob Level	Term R-Squared
Temp	4	5258.016	1314.504	64.65	0.015291	0.245605
Ratio	4	11044.6	2761.151	135.79	0.007324	0.515900
Height	4	3813.016	953.254	46.88	0.020994	0.178108
Total Error	5	2526.417	505.2833			0.118011
Lack of Fit	3	2485.75	828.5833	40.75	0.024047	0.116111
Pure Error	2	40.66667	20.33333			0.001900

This report tests the significance of each factor. This display actually shows two reports. The top is the regular ANOVA Section defined below. Note that the denominator of the F-Ratios is the Total Error Mean Square. The second report is identical to the top, except that the denominator of the F-Ratios is now the Pure Error Mean Square.

Factor

This line lists the factor being tested for deletion. All terms that include this factor are included in the test. In our example, the terms being tested are as follows:

<u>Factor</u>	<u>Individual Terms Referred To</u>
Temp	Temp, Temp x Ratio, Temp x Height, Temp x Temp.
Ratio	Ratio, Temp x Ratio, Ratio x Height, Ratio x Ratio.
Height	Height, Height x Ratio, Height x Temp, Height x Height.

Note that there is overlap in these terms (some cross-products occur twice).

DF

The degrees of freedom associated with the term(s).

Last Sum-Squares

The regression sum of squares that would be lost if this factor were omitted.

Mean Square

The sum of squares divided by the degrees of freedom.

F-Ratio

In the top report, the F-value is formed by dividing the Mean Square by the Total Error Mean Square. In the second report, the F-value is formed by dividing the Mean Square by the Pure Error Mean Square. Note that these tests are not sequential, but each tests the importance of the factor after considering all other factors.

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Prob Level

This is the right-tail probability or significance level of this test. Reject the hypothesis that the influence of the terms is zero when this value is less than a predetermined value of alpha, say 0.05.

Term R-Squared

The amount that the R-Squared would decrease if this factor were removed from the model.

Lack of Fit / Pure Error

These lines are only displayed if you have repeated observations from which the variability between like observations may be estimated. The lack of fit tests the adequacy of the specified model. If this test is significant, conclude that a higher order polynomial (such as cubic), or a different functional form, would fit the data better.

Estimation Section

Estimation Section						
Parameter	DF	Regression Coefficient	Standard Error	T-Ratio	Prob Level	Last R-Squared
Intercept	1	-30.66667				
Temp	1	-12.125	7.947353	-1.53	0.187613	0.054938
Ratio	1	-17	7.947353	-2.14	0.085417	0.107995
Height	1	-21.375	7.947353	-2.69	0.043321	0.170733
Temp^2	1	32.08333	11.69819	2.74	0.040667	0.177530
Ratio^2	1	47.83333	11.69819	4.09	0.009457	0.394616
Height^2	1	6.083333	11.69819	0.52	0.625242	0.006383
Temp*Ratio	1	8.25	11.23925	0.73	0.495884	0.012717
Temp*Height	1	1.5	11.23925	0.13	0.899034	0.000420
Ratio*Height	1	-1.75	11.23925	-0.16	0.882357	0.000572
Estimation Section Using Pure Error						
Parameter	DF	Regression Coefficient	Standard Error	T-Ratio	Prob Level	Last R-Squared
Intercept	1	-30.66667				
Temp	1	-12.125	1.594261	-7.61	0.016853	0.054938
Ratio	1	-17	1.594261	-10.66	0.008680	0.107995
Height	1	-21.375	1.594261	-13.41	0.005517	0.170733
Temp^2	1	32.08333	2.346688	13.67	0.005307	0.177530
Ratio^2	1	47.83333	2.346688	20.38	0.002398	0.394616
Height^2	1	6.083333	2.346688	2.59	0.122137	0.006383
Temp*Ratio	1	8.25	2.254625	3.66	0.067241	0.012717
Temp*Height	1	1.5	2.254625	0.67	0.574315	0.000420
Ratio*Height	1	-1.75	2.254625	-0.78	0.518860	0.000572

This report shows the regression coefficient estimates of each term and their test of significance. This display actually shows two reports. The top is the regular Estimation Section defined below. Note that the Standard Errors are based on the Total Error Mean Square. The second report is identical to the top, except that the Standard Errors are now based on the Pure Error Mean Square.

Parameter

The particular term being displayed.

DF

The degrees of freedom associated with the term.

Regression Coefficient

The estimated value of the regression coefficient.

Standard Error

The standard error of the above regression coefficient. Note that the Total Error Mean Square is used for the top report, and the Pure Error Mean Square is used for the bottom report.

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T-Ratio

The t-value for testing that this regression coefficient is zero after considering all other terms in the model. Note that the Total Error Mean Square is used for the top report, and the Pure Error Mean Square is used for the bottom report.

Prob Level

The probability or significance level of this test. If you were testing at the alpha equals 0.05 level of significance, this value would have to be less than 0.05 in order for the test to be deemed significant and the regression coefficient different from zero.

Last R-Squared

The amount that the R-Squared would decrease if this term were removed from the model.

Optimum Solution Section

Optimum Solution Section		
Parameter	Maximum Exponent	Optimum Value
Temp	2	0.1219125
Ratio	2	0.1995746
Height	2	1.770525
Function at optimum		-52.02463
Number of Function Evaluations		359
Maximum Functions Evaluations		500

This report gives the results of the function minimization (or maximization) calculation.

Optimum Value

The value for each of the factors at the computed critical point. Covariates were evaluated at their means. Note that this solution is not constrained to fall within the design space. Note also that the values of some variables may be very large or small. This indicates that the function did not have a minimum (maximum) and that the search procedure was terminated by the maximum number of function evaluations. In this case, you might switch from finding a minimum to finding a maximum in the Optimization Goal box.

Function at Optimum

The value of the estimated function evaluated at the optimal values of each of the factors.

Residual Section

Residual Section

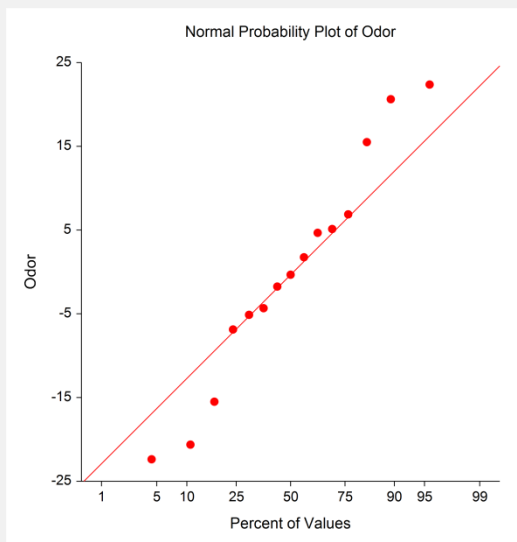
Row	Odor	Predicted	Residual
1	66	86.625	-20.625
2	58	42.5	15.5
3	65	59.875	5.125
4	-31	-30.66667	-.3333333
5	39	45.875	-6.875
6	17	15.25	1.75
7	7	29.375	-22.375
8	-35	-30.66667	-4.3333333
9	43	36.125	6.875
10	-5	-3.25	-1.75
11	43	20.625	22.375
12	-26	-30.66667	4.666667
13	49	28.375	20.625
14	-40	-24.5	-15.5
15	-22	-16.875	-5.125
16		28.375	

This report shows the response variable, the predicted value based on the response surface equation, and the residual (the difference between the two).

Notice that a predicted value is given for row sixteen, but no residual or Odor value is given. If you look at row sixteen on the database, you will note that it has a missing value for Odor and thus was not used in estimating the regression equation. However, since there are values for the three independent variables, a predicted value can be generated. This shows how to automatically generate predicted values for a set of X's when the observed Y is not on your database.

Normal Probability Plot

This plot displays a normal probability plot for assessing the validity of the assumption of normality. Note that you should ignore this plot when you have less than about five observations per term in the model, since the assumption of independence of residuals cannot be demonstrated and thus the probability plot may give inaccurate results.



Response Surface Regression

Contour Plot

This contour (or grid) plot shows the value of the estimated equation at the center of each grid of rectangles. All factors not on either axis are evaluated at their mean value (unless a constant value was specified in the Factor Constant box).

