

Chapter 450

Clustered Heat Maps (Double Dendrograms)

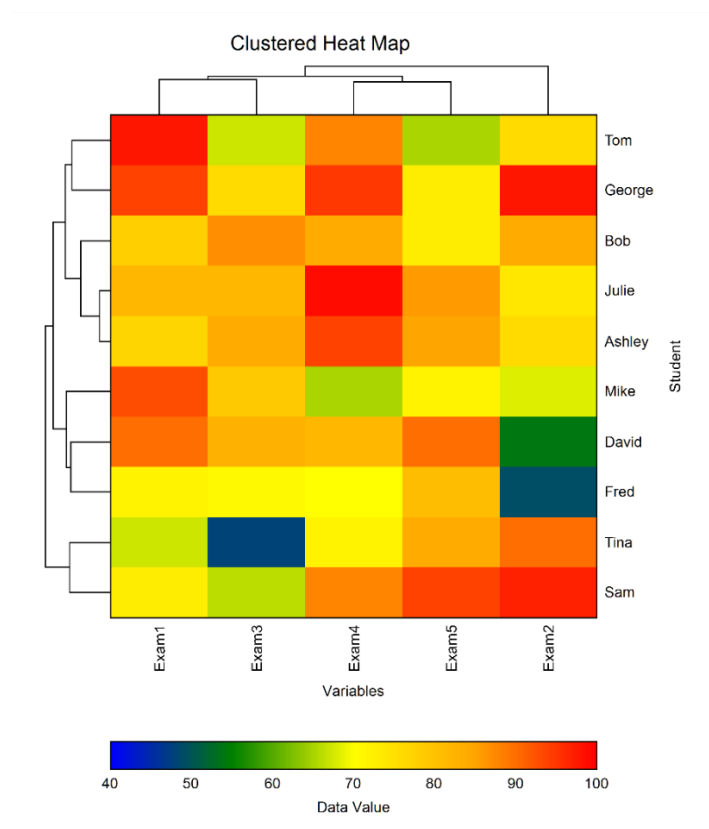
Introduction

This chapter describes how to obtain a clustered heat map (sometimes called a double dendrogram) using the Clustered Heat Map procedure.

Similar to a contour plot, a heat map is a two-way display of a data matrix in which the individual cells are displayed as colored rectangles. The color of a cell is proportional to its position along a color gradient. Usually, the columns (variables) of the matrix are shown as the columns of the heat map and the rows of the matrix are shown as the rows of the heat map, as in the example below. The order of the rows is determined by performing hierarchical cluster analyses of the rows. This tends to position similar rows together on the plot. The order of the columns is determined similarly.

Usually, a clustered heat map is made on variables that have similar scales, such as scores on tests in the example below. If the variables have different scales, the data matrix must first be scaled using a standardization transformation such as z-scores or proportion of the range.

Here is an example of a clustered heat map.



Hierarchical Clustering Algorithms

The cluster algorithms used for the rows and columns of the data matrix must be specified. NCSS allows you to select from eight possible hierarchical algorithms. The clustering method selected for the columns need not be the same as the method selected for the rows. Chapter 445 of the *NCSS* documentation gives an introduction to hierarchical clustering. Only highlights from that chapter are presented here.

We will first give brief comments about each of the eight hierarchical clustering techniques.

Group Average

Also called the unweighted pair-group method, this is perhaps the most widely used of all the hierarchical cluster techniques. The distance between two groups is defined as the average distance between each of their members.

Single Linkage

Also known as *nearest neighbor* clustering, this is one of the oldest and most famous of the hierarchical techniques. The distance between two groups is defined as the distance between their two closest members. It often yields clusters in which individuals are added sequentially to a single group.

Complete Linkage

Also known as furthest neighbor or maximum method, this method defines the distance between two groups as the distance between their two farthest-apart members. This method usually yields clusters that are well separated and compact.

Simple Average

Also called the weighted pair-group method, this algorithm defines the distance between groups as the average distance between each of the members, weighted so that the two groups have an equal influence on the final result.

Centroid

Also referred to as the unweighted pair-group centroid method, this method defines the distance between two groups as the distance between their centroids (center of gravity or vector average). The method should only be used with Euclidean distances.

Backward links may occur with this method. These are recognizable when the dendrogram no longer exhibits its simple tree-like structure in which each fusion results in a new cluster that is at a higher distance level (moves from right to left). With backward links, fusions can take place that result in clusters at a lower distance level (move from left to right). The dendrogram is difficult to interpret in this case.

Median

Also called the weighted pair-group centroid method, this defines the distance between two groups as the weighted distance between their centroids, the weight being proportional to the number of individuals in each group. Backward links (see discussion under Centroid) may occur with this method. The method should only be used with Euclidean distances.

Ward's Minimum Variance

With this method, groups are formed so that the pooled within-group sum of squares is minimized. That is, at each step, the two clusters are fused which result in the least increase in the pooled within-group sum of squares.

Clustered Heat Maps (Double Dendrograms)

Flexible Strategy

Lance and Williams (1967) suggested that a continuum could be made between single and complete linkage. The program lets you try various settings of these parameters which do not conform to the constraints suggested by Lance and Williams.

One interesting exercise is to vary these values, trying to find the set that maximizes the cophenetic correlation coefficient.

Goodness-of-Fit

Given the large number of techniques, it is often difficult to decide which is best. One criterion that has become popular is to use the result that has largest *cophenetic correlation coefficient*. This is the correlation between the original distances and those that result from the cluster configuration. Values above 0.75 are felt to be good. The Group Average method appears to produce high values of this statistic. This may be one reason that it is so popular.

A second measure of goodness of fit called *delta* is described in Mather (1976). These statistics measure degree of distortion rather than degree of resemblance (as with the cophenetic correlation). The two delta coefficients are given by

$$\Delta_A = \left[\frac{\sum_{j < k}^N |d_{jk} - d_{jk}^*|^{1/A}}{\sum_{j < k} (d_{jk}^*)^{1/A}} \right]^A$$

where A is either 0.5 or 1 and d_{ij}^* is the distance obtained from the cluster configuration. Values close to zero are desirable.

Mather (1976) suggests that the Group Average method is the safest to use as an exploratory method, although he goes on to suggest that several methods should be tried and the one with the largest cophenetic correlation be selected for further investigation.

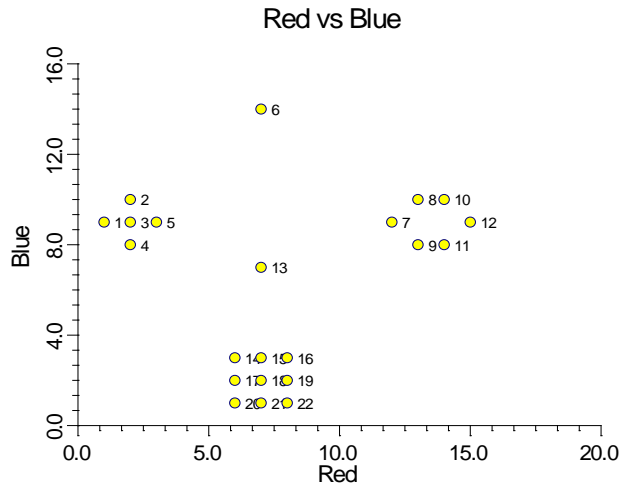
Dendrograms

The *agglomerative hierarchical clustering* algorithms available in this program module build a cluster hierarchy that is commonly displayed as a tree diagram called a *dendrogram*. The algorithm begins by placing each object in a separate cluster. Then, at each step, the two clusters that are most similar (according to a specific definition of similarity) are joined into a single new cluster. Once fused, objects are never separated. The eight clustering methods that are available represent eight methods of defining the similarity between clusters.

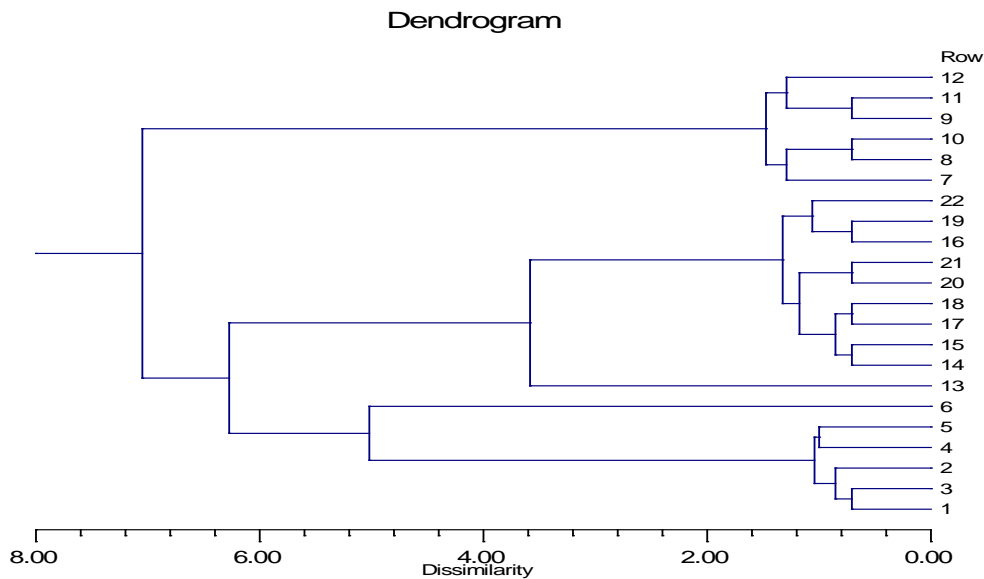
To help understand the dendrogram, consider the following example that has only two variables. Note that if we had only two variables, we could perform the cluster analysis visually. The technique becomes useful once we have three or more variables to consider.

Clustered Heat Maps (Double Dendrograms)

Suppose we wish to cluster the bivariate data shown in the following scatter plot. In this case, the clustering may be done visually. The data seem to exhibit three clusters and two singletons, 6 and 13.



The following dendrogram was produced from the above data using popular the Group Average clustering algorithm.



The horizontal axis of the dendrogram represents the distance or dissimilarity between clusters. The vertical axis represents the objects and clusters. The dendrogram is fairly simple to interpret. Remember that our main interest is in similarity and clustering. Each joining (fusion) of two clusters is represented on the graph by the splitting of a horizontal line into two horizontal lines. The horizontal position of the split, shown by the short vertical bar, gives the dissimilarity between the two clusters.

Looking at this dendrogram, you can see the three clusters as three branches that occur at about the same horizontal distance. The two outliers, 6 and 13, are added in rather arbitrarily at much higher distances. This is the interpretation.

In this example we can compare our interpretation with an actual plot of the data. Unfortunately, this usually will not be possible because our data will consist of more than two variables.

Missing Values

When an observation has missing values, appropriate adjustments are made so that the average dissimilarity across all variables with non-missing data is computed. Hence, rows with missing values are not omitted unless all variables have missing values. Note that the distances require that at least one variable have non-missing values for each pair of rows.

Example 1 – Creating a Clustered Heat Map

This section presents an example of how to create a clustered heat map from a set of exam score data. The data are found in the Exams database.

Setup

To run this example, complete the following steps:

1 Open the Exams example dataset

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

2 Specify the Clustered Heat Maps (Double Dendrograms) procedure options

- Find and open the **Clustered Heat Maps (Double Dendrograms)** 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.

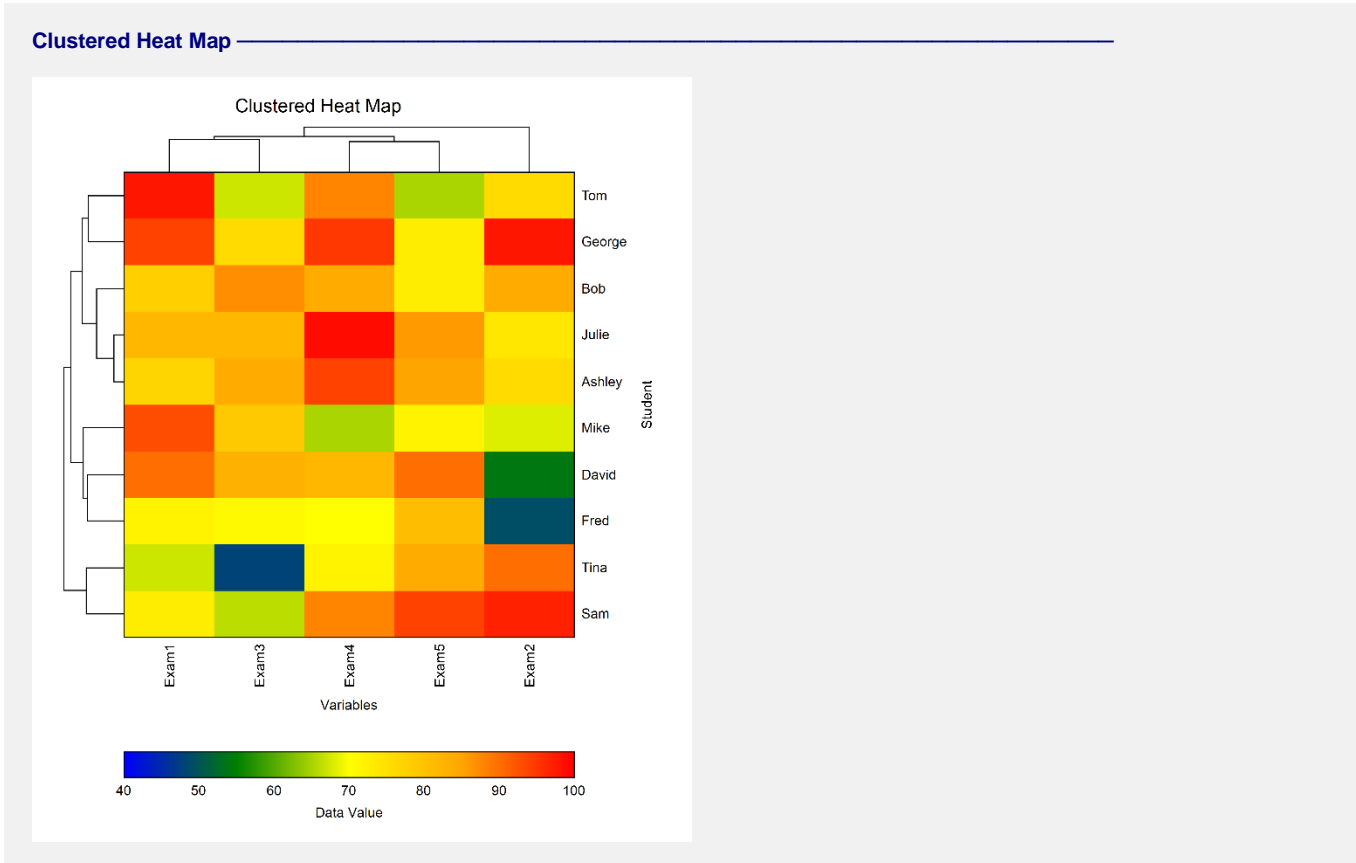
<u>Option</u>	<u>Value</u>
Variables Tab	
Cluster Variable(s)	Exam1, Exam2, Exam3, Exam4, Exam5
Row Label Variable	Student
Variable Scaling Method.....	None
Row Scaling Method.....	None
Reports Tab	
Clustered Heat Map.....	Checked
Cluster Reports.....	Checked
Linkage Reports.....	Checked
Distance Reports	Checked

3 Run the procedure

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

Clustered Heat Maps (Double Dendrograms)

Heat Map Section



This report displays the heat map for these data with the above settings. Note that the rows and columns have been sorted in the order specified by the clustering.

Cluster Detail Section

Cluster Detail Report when Clustering Variables

Clustering Method Simple Average
 Distance Type Euclidean
 Scale Type None

Cluster	Variables in this Cluster
1	Exam1, Exam3
2	Exam4, Exam5
None	Exam2

Cluster Detail Report when Clustering Rows

Clustering Method Simple Average
 Distance Type Euclidean
 Scale Type None

Cluster	Rows in Cluster
1	Tom, Bob, Julie, Ashley, George
2	Tina, Sam
3	Mike, David, Fred

This report displays the items contained in the row and variable clusters. Those items that cannot be classified are listed in the 'None' cluster.

Linkage Section

Linkage Report when Clustering Variables

Clustering Method Simple Average
 Distance Type Euclidean
 Scale Type None

Link	Number Clusters	Distance Value	Distance Bar
4	1	19.413274	
3	2	15.493208	
2	3	14.390969	
1	4	13.408952	

Cophenetic Correlation 0.829879
 Delta(0.5) 0.067471
 Delta(1.0) 0.090232

Linkage Report when Clustering Rows

Clustering Method Simple Average
 Distance Type Euclidean
 Scale Type None

Link	Number Clusters	Distance Value	Distance Bar
9	1	19.763410	
8	2	17.446811	
7	3	13.832703	
6	4	13.428924	
5	5	12.369317	
4	6	11.983322	
3	7	11.781341	
2	8	9.159521	
1	9	3.435113	

Cophenetic Correlation 0.765894
 Delta(0.5) 0.125960
 Delta(1.0) 0.178253

This report displays the number of clusters that exist at each link. The links are displayed in reverse order so that you can quickly determine an appropriate number of clusters to use. It displays the distance level at which the fusion took place. It will let you precisely determine the best value of the number of clusters.

The cophenetic correlation and two delta goodness of fit statistics are reported at the bottom of this report. As discussed earlier, these values let you compare the fit of various cluster configurations.

Link

This is the sequence number of the fusion.

Number Clusters

This is the number of clusters that would result if the cluster cutoff value were set to the corresponding Distance Value or higher. Note that this number includes outliers.

Distance Value

This is distance value between the two joining clusters that is used by the algorithm. Normally, this value is monotonically increasing. When backward linking occurs, this value will no longer exhibit a strictly increasing behavior.

Distance Bar

This is a bar graph of the Distance Values. Choose the number of clusters by finding a jump in the decreasing pattern shown in this bar chart.

Clustered Heat Maps (Double Dendrograms)

Cophenetic Correlation

This is the Pearson correlation between the actual distances and the predicted distances based on this particular hierarchical configuration. A value of 0.75 or above needs to be achieved in order for the clustering to be considered useful.

Delta (0.5, 1)

These are the values of the goodness of fit deltas. When comparing to clustering configurations, the configuration with the smallest delta value fits the data better.

Distance Section

Distance Report when Clustering Variables					
Clustering Method		Simple Average			
Distance Type		Euclidean			
Scale Type		None			
First Row	Second Row	Actual Distance	Dendrogram Distance	Actual Difference	Percent Difference
1	2	20.386270	19.413274	0.972996	4.77
1	3	14.390969	14.390969	0.000000	0.00
1	4	13.479614	15.493208	-2.013593	-14.94
1	5	16.991174	15.493208	1.497966	8.82
2	3	22.074873	19.413274	2.661599	12.06
2	4	16.555966	19.413274	-2.857308	-17.26
2	5	18.635987	19.413274	-0.777287	-4.17
3	4	15.678010	15.493208	0.184802	1.18
3	5	15.824032	15.493208	0.330825	2.09
4	5	13.408952	13.408952	0.000000	0.00
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.
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This report displays the actual and predicted distance for each pair of variables (and, later, rows). It also includes their difference and percent difference. Since the report grows very long for even a modest number of rows, it is often omitted.

Example 2 – Creating a Clustered Heat Map with only Two Colors

This section presents an example of how to create a clustered heat map of the exam score data with a gradient of just two colors. The data are found in the Exams database.

Setup

To run this example, complete the following steps:

1 Open the Exams example dataset

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

2 Specify the Clustered Heat Maps (Double Dendrograms) procedure options

- Find and open the **Clustered Heat Maps (Double Dendrograms)** procedure using the menus or the Procedure Navigator.
- The settings for this example are listed below and are stored in the **Example 2** 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	
Cluster Variable(s)	Exam1, Exam2, Exam3, Exam4, Exam5
Row Label Variable	Student
Variable Scaling Method.....	None
Row Scaling Method.....	None

Reports Tab

Clustered Heat Map.....	Checked
Cluster Reports.....	Unchecked
Linkage Reports.....	Unchecked
Distance Reports	Unchecked

Clustered Heat Map Format (*Click the Button*)

Heat Map Tab

Data Gradient Fill Format (*Click the Button*)

Remove the center three stops so that there are only a blue and a red stop showing. Stops are removed by selecting them and then pressing the **Remove** button.

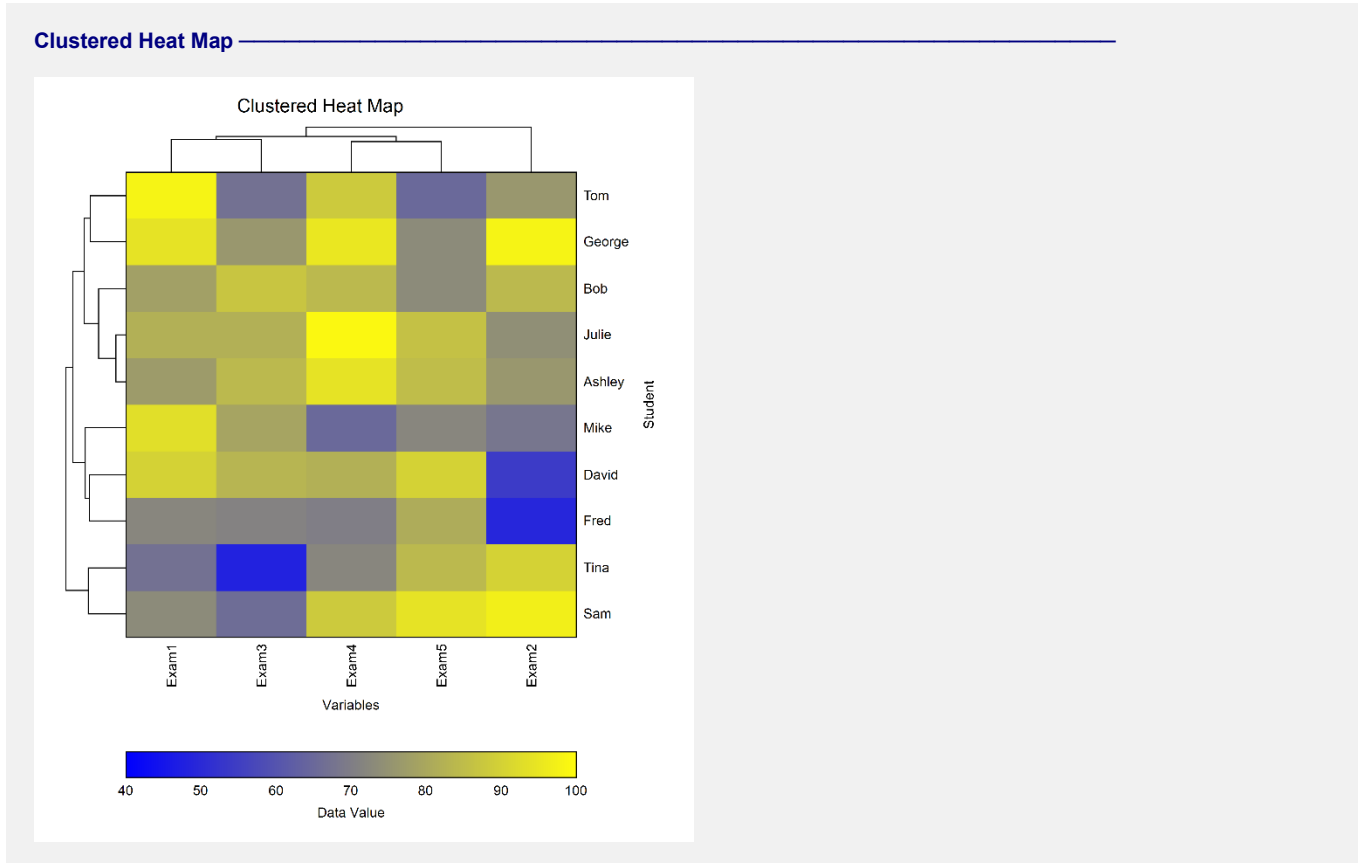
Select the **Red (right)** button. **Change the color to yellow** by clicking on the **Color** button which is just below the **Remove** button.

3 Run the procedure

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

Clustered Heat Maps (Double Dendrograms)

Output



This report displays the heat map for these data with the above settings.

Example 3 – Creating a Clustered Heat Map with Slanted Labels

This section presents an example of how to create a clustered heat map of the exam score data with a gradient of just two colors and with slanted row labels down the right side of the plot. The data are found in the Exams database.

Setup

To run this example, complete the following steps:

1 Open the Exams example dataset

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

2 Specify the Clustered Heat Maps (Double Dendrograms) procedure options

- Find and open the **Clustered Heat Maps (Double Dendrograms)** procedure using the menus or the Procedure Navigator.
- The settings for this example are listed below and are stored in the **Example 3** settings template. To load this template, click **Open Example Template** in the Help Center or File menu.

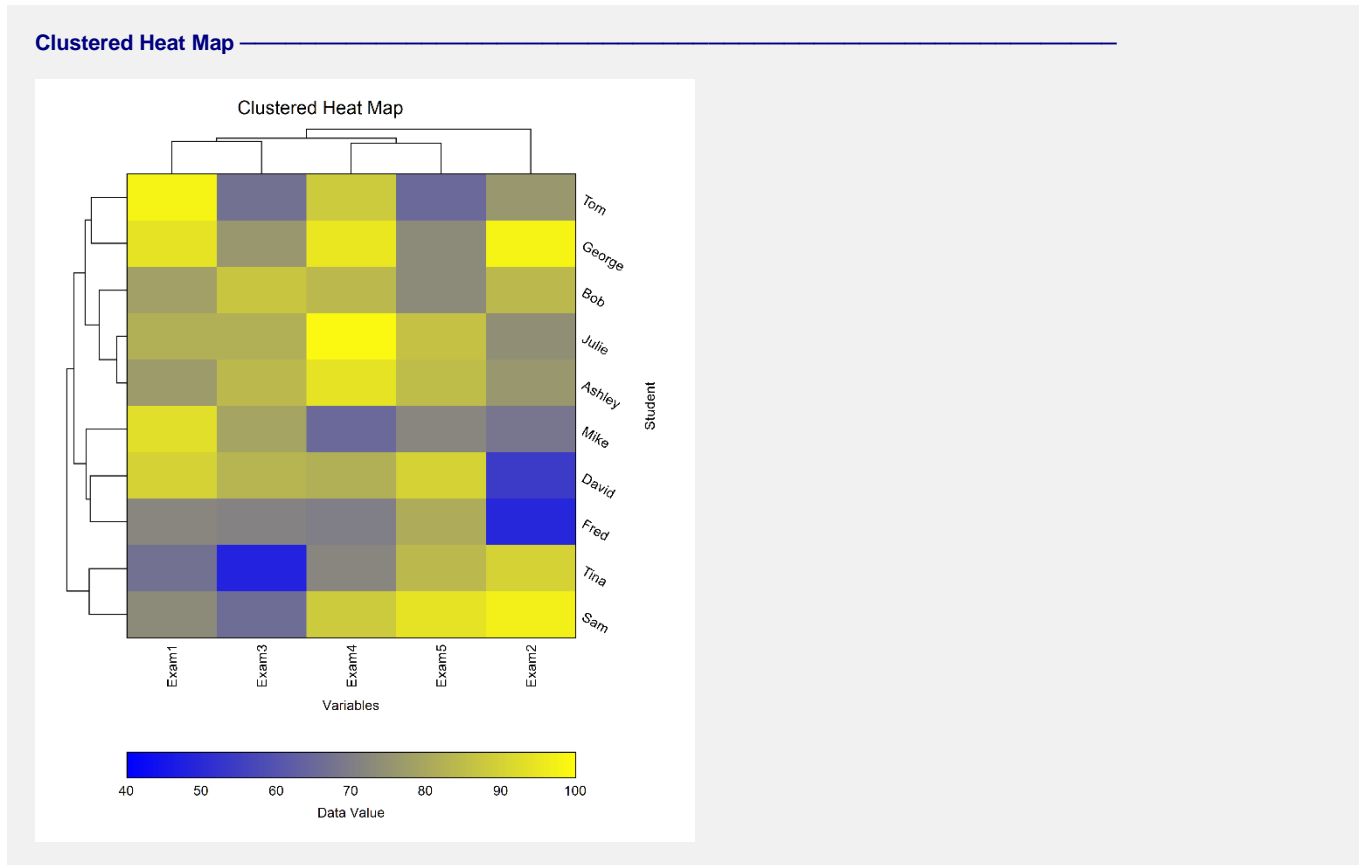
<u>Option</u>	<u>Value</u>
Variables Tab	
Cluster Variable(s)	Exam1, Exam2, Exam3, Exam4, Exam5
Row Label Variable	Student
Variable Scaling Method.....	None
Row Scaling Method.....	None
Reports Tab	
Clustered Heat Map.....	Checked
Cluster Reports.....	Unchecked
Linkage Reports.....	Unchecked
Distance Reports	Unchecked
Clustered Heat Map Format (<i>Click the Button</i>)	
<i>Heat Map Tab</i>	
Data Gradient Fill Format (<i>Click the Button</i>)	
Remove the center three stops so that there are only a blue and a red stop showing. Stops are removed by selecting them and then pressing the Remove button.	
Select the Red (right) button. Change the color to yellow by clicking on the Color button which is just below the Remove button.	
Tick Labels – Rows Format (<i>Click the Button</i>)	
Angle	-30

3 Run the procedure

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

Clustered Heat Maps (Double Dendrograms)

Output



This report displays the heat map for these data with the above settings.