

Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise. Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix	Name of Variable Matrix	Name of Filename Matrix	Name of Totalcounts Matrix	Name of Samplenames Matrix
Select Data	Select Variables	Select Filenames	Select Totalcounts	Select Samples

This tutorial contains navigation buttons that enable you to move throughout the tutorial.

Please use the navigation buttons and not the page up/page down or arrow keys to navigate through the tutorials.

This is the 'Next' button. It takes you to the next frame or stop point.



This is the 'Previous' button. It takes you to the previous frame or stop point.



This is the 'Go to frame' button. It takes you to a specified frame.



This is the 'Go to URL' button. It takes you to a website link.



Press the 'Next' button below to start this tutorial.



Workspace



Name

data
exactmass
filenames
ndatass
nommass
ntestdatass
samplenames
testdata
testfiles
testsamples
totalcounts

Current Directory Workspace

Command History

-----%-- 10/8/10 10:49

Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise.
Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix

ndatass

Name of Variable Matrix

exactmass

Name of Filename Matrix

filenames

Name of Totalcounts Matrix

totalcounts

Name of Samplenames Matrix

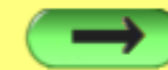
samplenames

This tutorial will show how to create a PCA model and then project new data into the model.

For this we will use the 'Run PCA' function to create and save the model and then the 'PCA Modelling' function to project the new data into the model.

Before doing this procedure you will need to have a data set for building the model and a separate data set that you want to project into the model.

Each set of data needs to have it's own list of files and samplenames.





Workspace



- Name
- data
- exactmass
- filenames
- ndatass
- nommass
- ntestdatass
- samplenames
- testdata
- testfiles
- testsamples
- totalcounts

Command History

```
---%-- 10/8/10 10:49
```

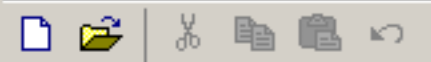
Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise. Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix	Name of Variable Matrix	Name of Filename Matrix	Name of Totalcounts Matrix	Name of Samplenames Matrix
ndatass	exactmass	filenames	totalcounts	samplenames

First we need to build a PCA model.

← →



Workspace

- Name
- data
- exactmass
- filenames
- ndatass
- nommass
- ntestdatass
- samplenames
- testdata
- testfiles
- testsamples
- totalcounts

Command History

```
---%-- 10/8/10 10:49
```

- Run PCA
- PCA Modelling
- Run DPCA
- Export MVA Data

From the 'MVA' menu choose -> 'Run PCA'

Name of Data Matrix	Name of Variable Matrix	Name of Filename Matrix	Name of Totalcounts Matrix	Name of Samplenames Matrix
ndatass	exactmass	filenames	totalcounts	samplenames

File Edit Debug Desktop

Shortcuts How to Add

Workspace

Name

- data
- exactmass
- filenames
- ndatass
- nommass
- ntestdatass
- samplenames
- testdata
- testfiles
- testsamples
- totalcounts

Current Directory Workspace

Command History

```
----%-- 10/8/10 10:49
```

Data Selection Panel

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Name of Data Matrix	Name of Variable Matrix	Name of Filename Matrix	Name of Totalcounts Matrix	Name of Samplenames Matrix
ndatass	exactmass	filenames	totalcounts	samplenames

PCA Panel

Input Information

Make sure the data selected above is the data you want to use.

Make sure the correct set of data is loaded with the correct filename and samplename list.



Load Selected Data

Data:	None
Samples:	None
Variables:	None

Scaling Method

Choose one

Run PCA

Show Eigenvalue Scree Plot

PCA Summary

PC#	%Var	%Vartotal

Close Panel



Workspace

- Name
- data
- exactmass
- filenames
- ndatass
- nommass
- ntestdatass
- samplenames
- testdata
- testfiles
- testsamples
- totalcounts

Command History

```

>> %-- 10/8/10 10:49

```

Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise. Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix:
 Name of Variable Matrix:
 Name of Filename Matrix:
 Name of Totalcounts Matrix:
 Name of Samplenames Matrix:

PCA Panel

Input Information

Make sure the data selected above is the data you want to analyze and then press the "Load Selected Data" button.

Load Selected Data

Data: **ndatass**
 Samples: **samplenames**
 Variables: **exactmass**

Scaling Method

Choose one

Run PCA

Show Eigenvalue Scree Plot

PCA Summary

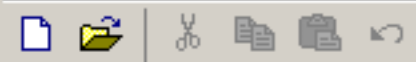
PC#	%Var	%Vartotal

Choose the scaling/preprocessing you would like to use.

NOTE: The choice you make here is automatically applied to the new data when it is projected into the PCA model.

← →

Close Panel



Shortcuts How to Add

Workspace



Name

- data
- exactmass
- filenames
- ndatass
- nommass
- ntestdatass
- samplenames
- testdata
- testfiles
- testsamples
- totalcounts

Current Directory Workspace

Command History

```
----%-- 10/8/10 10:49
```

Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise. Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix ndatass	Name of Variable Matrix exactmass	Name of Filename Matrix filenames	Name of Totalcounts Matrix totalcounts	Name of Samplenames Matrix samplenames
---------------------------------------	---	---	--	--

PCA Panel

Input Information

Make sure the data selected above is the data you want to analyze and then press the "Load Selected Data" button.

Load Selected Data

Data: ndatass
Samples: samplenames
Variables: exactmass

Scaling Method

Mean Center

Run PCA

Press the 'Run PCA' button.

← →

Show Eigenvalue Scree Plot

PCA Summary

PC#	%Var	%Vartotal

Close Panel

Workspace

Name
data
exactmass
filenames
ndatass
nommass
ntestdatass
samplenames
testdata
testfiles
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totalcounts

Data Selection Panel

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Name of Data Matrix: Name of Variable Matrix: Name of Filename Matrix: Name of Totalcounts Matrix: Name of Samplenames Matrix:

Input Information

Make sure the data selected above is the data you want to analyze and then press the "Load Selected Data" button.

Load Selected Data

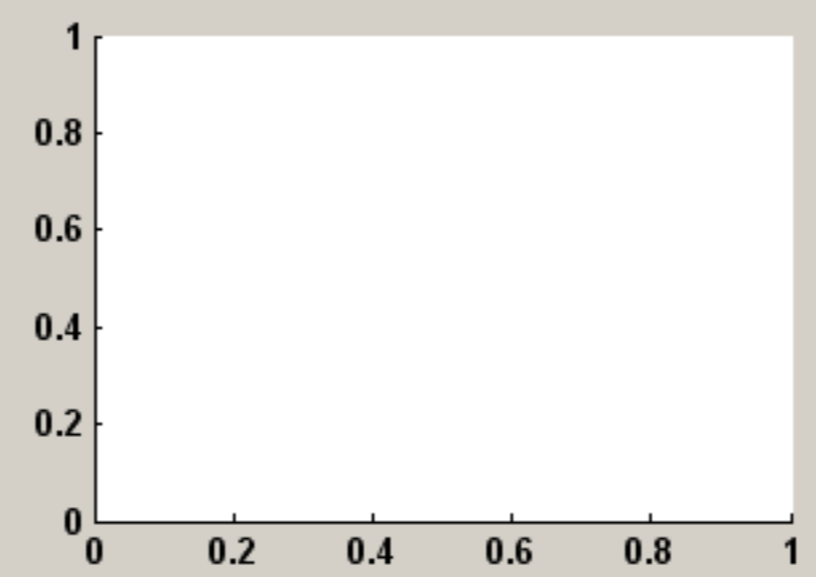
PCA Panel

Plot PCA Scores and Loadings

These plots are for a quick check of the results and cannot be saved.

Loading plots default to m/z vs PC#.

PC# PC#
 Plot Scores Plot Loads



Save PCA Data to Workspace

Number of PCs to keep

Scores output name

Loadings output name

Percent variance output name

Model output name

Save To Workspace

Close Panel

When creating a PCA model the number of PCs kept in the model is very important. Selecting too few PCs will create a model that may not have good predictive ability, selecting too many PCs will create a model that is too restrictive to the calibration set and that will be modelling noise.

For this data set looking at the % variance it looks like the numbers stop changing significantly around PC 7 or 8.

PCA Summary

PC#	%Var	%Vartotal
1	52.3	52.3
2	20.6	73
3	13.7	86.7
4	7.1	93.8
5	3.5	97.2
6	1.5	98.8
7	1	99.7
8	0.1	99.8
9	0.1	99.9
10	0	99.9

Workspace

Name ▲

- data
- exactmass
- filenames
- ndatass
- nommass
- ntestdatass
- samplenames
- testdata
- testfiles
- testsamples
- totalcounts

Current Directory Workspace

Command History

```

>> 10/8/10 10:49

```

Data Selection Panel

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Name of Data Matrix: Name of Variable Matrix: Name of Filename Matrix: Name of Totalcounts Matrix: Name of Samplenames Matrix:

Input Information

Make sure the data selected above is the data you want to analyze and then press the "Load Selected Data" button.

Load Selected Data

Data: **ndatass**
 Samples: **samplenames**
 Variables: **exactmass**

Scaling Method

Run PCA

Show Eigenvalue Scree Plot

PCA Summary

PC#	%Var	%Vartotal
1	52.3	52.3
2	20.6	73
3	13.7	86.7
4	7.1	93.8
5	3.5	97.2
6	1.5	98.8
7	1	99.7
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9	0.1	99.9
10	0	99.9

PCA Panel

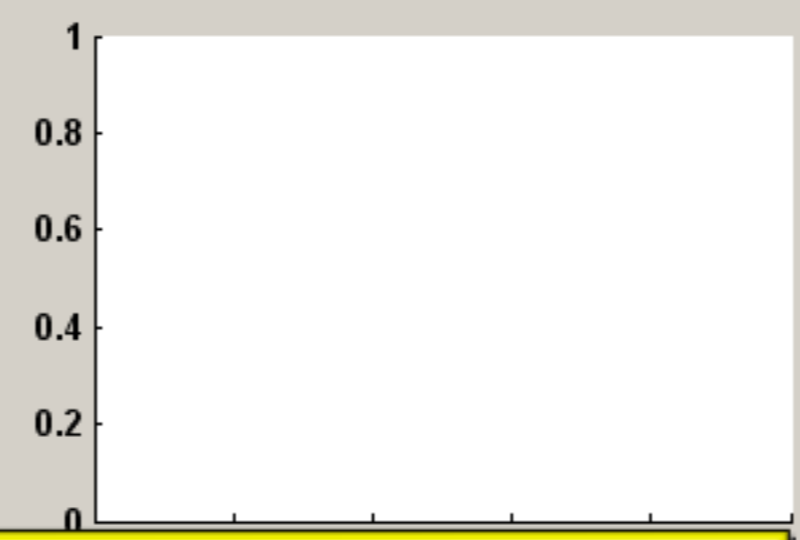
Plot PCA Scores and Loadings

These plots are for a quick check of the results and cannot be saved.

Loading plots default to m/z vs PC#.

PC# PC#

Plot Scores Plot Loads



Save PCA Data to Workspace

Number of PCs to keep:

Scores output name:

Loadings output name:

Percent variance output name:

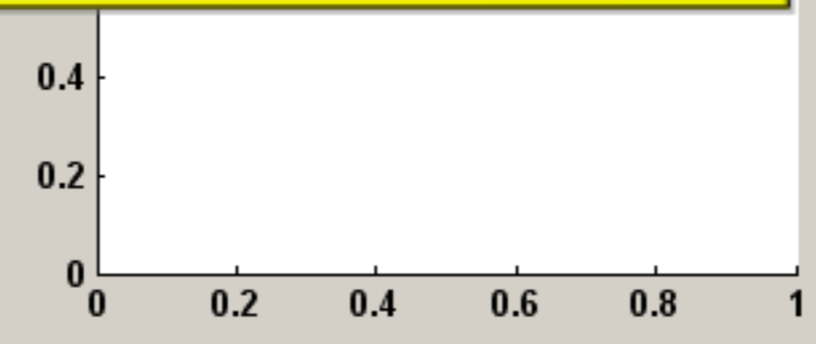
Model output name:

Save To Workspace

Close Panel

Let's see what the scree plot looks like. Press the 'Show Eigenvalue Scree Plot' button.

← →





Workspace



Name

- data
- exactmass
- filenames
- ndatass
- nommass
- ntestdatass
- samplenames
- testdata
- testfiles
- testsamples
- totalcounts

Current Directory Workspace

Command History

---%-- 10/8/10 10:49

Data Selection Panel

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Name of Data Matrix: Name of Variable Matrix: Name of Filename Matrix: Name of Totalcounts Matrix: Name of Samplenames Matrix:

Input Information

Make sure the data selected above is the data you want to analyze and then press the "Load Selected Data" button.

Load Selected Data

Data: **ndatass**
 Samples: **samplenames**
 Variables: **exactmass**

Scaling Method

Mean Center

PCA Panel

Plot PCA Scores and Loadings

These plots are for a quick check of the results and cannot be saved.

Loading plots default to m/z vs PC#.

PC# PC#
 Plot Scores Plot Loads

Save PCA Data to Workspace

Number of PCs to keep

Scores output name

Loadings output name

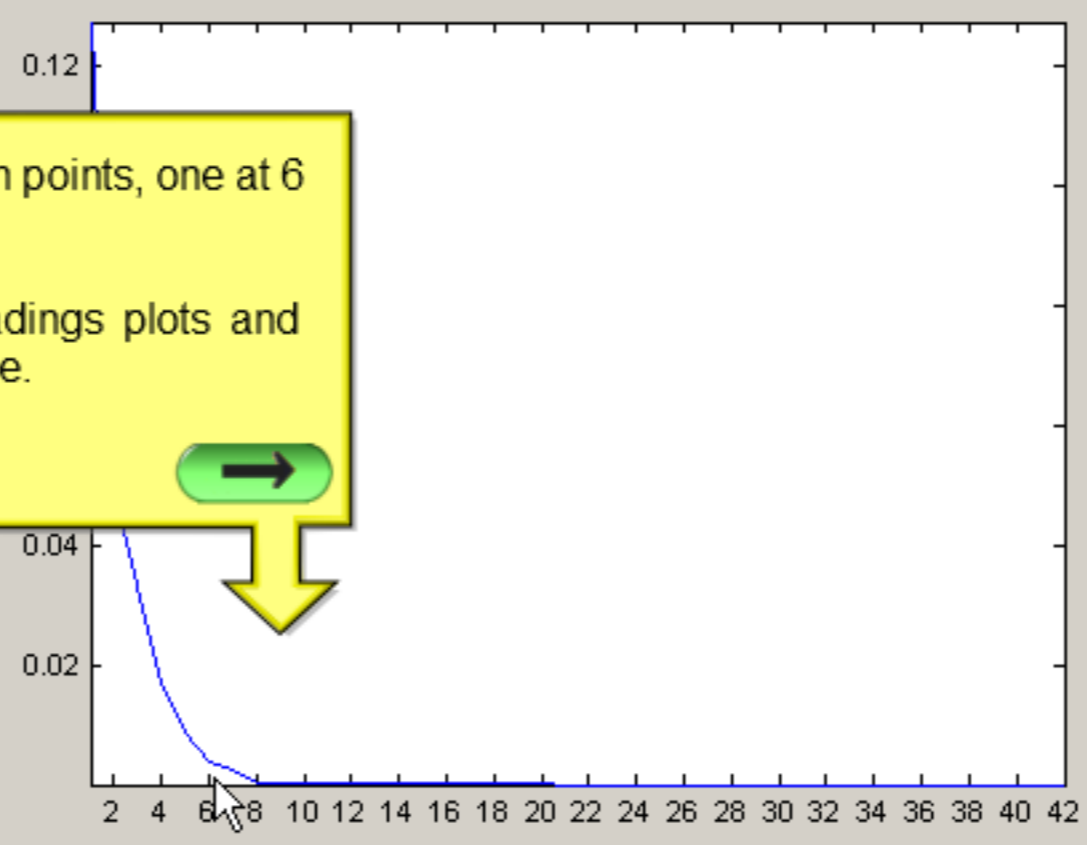
Percent variance output name

Model output name

Save To Workspace

Close Panel

Eigenvalue Scree Plot

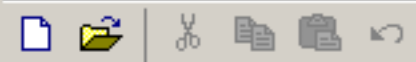


It looks like there are two inflection points, one at 6 and one at 8.

Let's look at the scores and loadings plots and see what PCs 6 through 8 look like.

1	52.3	52.3
2	20.6	73
3	13.7	86.7
4	7.1	93.8
5	3.5	97.2
6	1.5	98.8
7	1	99.7
8	0.1	99.8
9	0.1	99.9
10	0	99.9

Close



Shortcuts How to Add

Workspace



Name

- data
- exactmass
- filenames
- ndatass
- nommass
- ntestdatass
- samplenames
- testdata
- testfiles
- testsamples
- totalcounts

Current Directory Workspace

Command History

---%-- 10/8/10 10:49

Data Selection Panel

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Name of Data Matrix: **ndatass** | Name of Variable Matrix: **exactmass** | Name of Filename Matrix: **filenames** | Name of Totalcounts Matrix: **totalcounts** | Name of Samplenames Matrix: **samplenames**

Input Information

Make sure the data selected above is the data you want to analyze and then press the "Load Selected Data" button.

Load Selected Data

Data: **ndatass**
 Samples: **samplenames**
 Variables: **exactmass**

Scaling Method
Mean Center

Run PCA

Show Eigenvalue Scree Plot

PCA Summary

PC#	%Var	%Vartotal
1	52.3	52.3
2	20.6	73
3	13.7	86.7
4	7.1	93.8
5	3.5	97.2
6	1.5	98.8
7	1	99.7
8	0.1	99.8
9	0.1	99.9
10	0	99.9

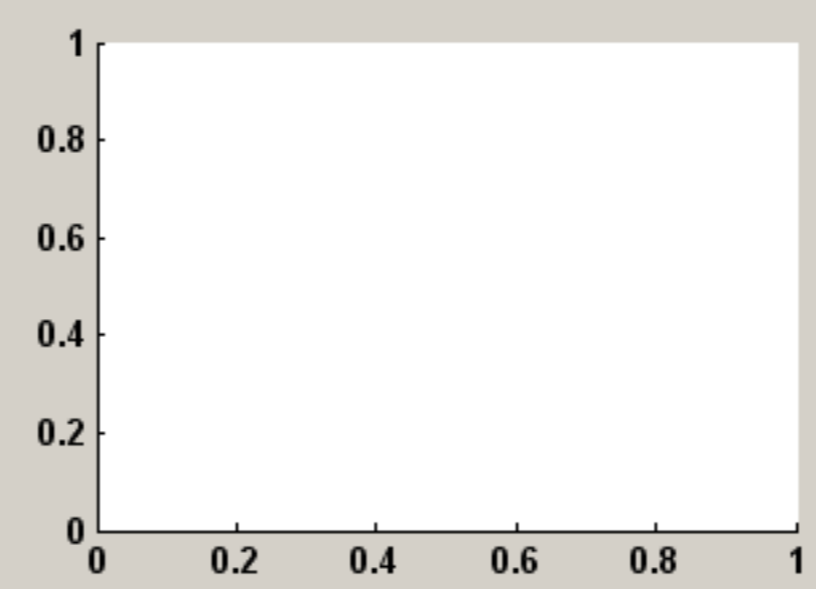
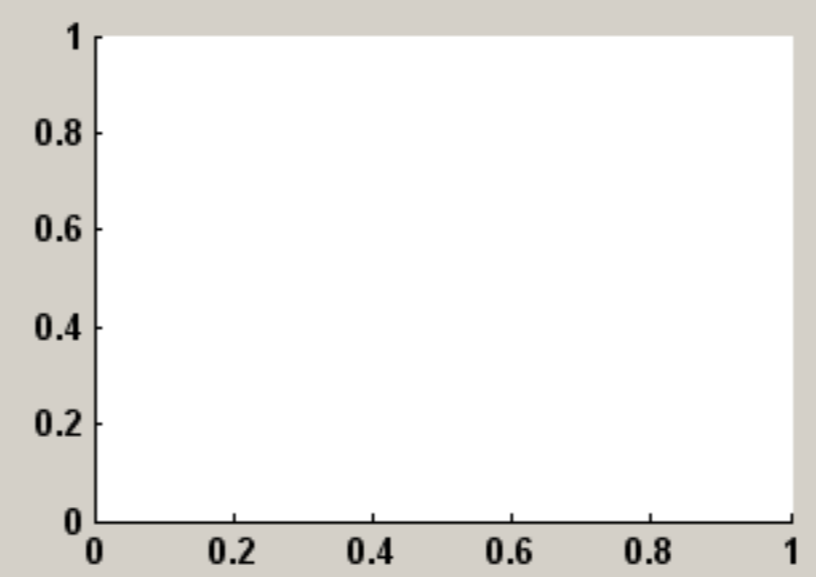
PCA Panel

Plot PCA Scores and Loadings

These plots are for a quick check of the results and cannot be saved.

Loading plots default to m/z vs PC#.

PC# [] | PC# []
 Plot Scores | Plot Loads



Save PCA Data to Workspace

Number of PCs to keep

First we'll look at PC 6.

← →

Percent variance output name

Model output name

Save To Workspace

Close Panel

Workspace

- Name ▲
- data
- exactmass
- filenames
- ndatass
- nommass
- ntestdatass
- samplenames
- testdata
- testfiles
- testsamples
- totalcounts

Current Directory Workspace

Command History

---%-- 10/8/10 10:49

Data Selection Panel

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Name of Data Matrix: Name of Variable Matrix: Name of Filename Matrix: Name of Totalcounts Matrix: Name of Samplenames Matrix:

Input Information

Make sure the data selected above is the data you want to analyze and then press the "Load Selected Data" button.

Load Selected Data

Data: **ndatass**
 Samples: **samplenames**
 Variables: **exactmass**

Scaling Method

Mean Center

Run PCA

Show Eigenvalue Scree Plot

PCA Summary

PC#	%Var	%Vartotal
1	52.3	52.3
2	20.6	73
3	13.7	86.7
4	7.1	93.8
5	3.5	97.2
6	1.5	98.8
7	1	99.7
8	0.1	99.8
9	0.1	99.9
10	0	99.9

PCA Panel

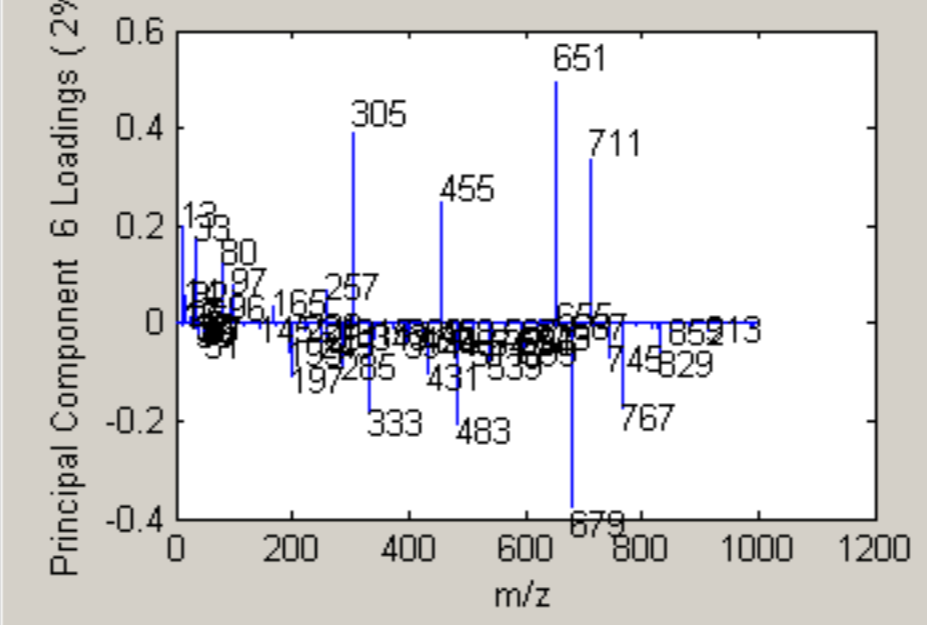
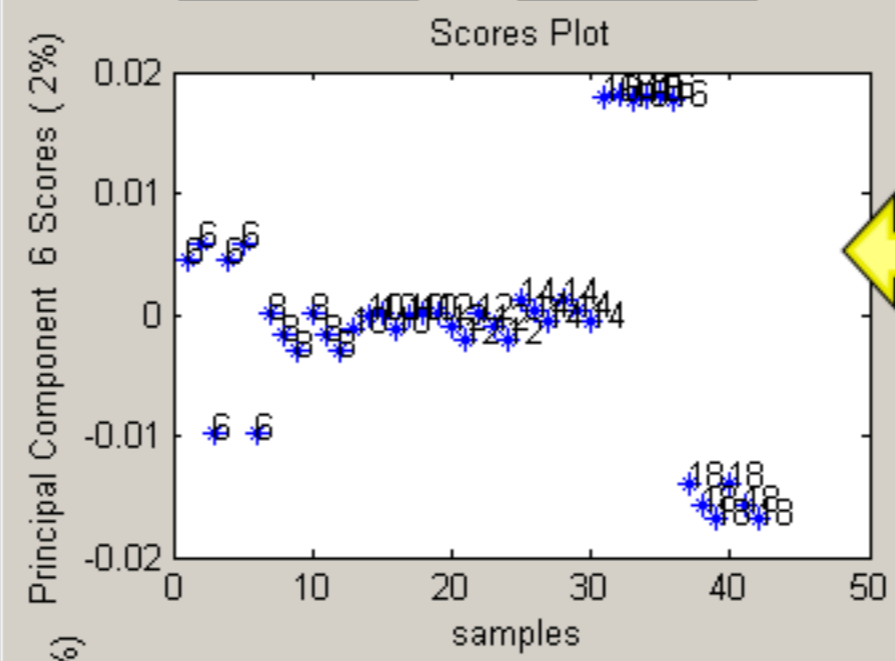
Plot PCA Scores and Loadings

These plots are for a quick check of the results and cannot be saved.

Loading plots default to m/z vs PC#.

samp/var

Plot Scores Plot Loads



Save PCA Data to Workspace

Number of PCs to keep

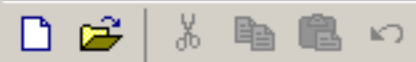
Scores output name

Loadings output name

Save To Workspace

Close Panel

It looks like PC6 separates the 16 and 18 samples. So there is some information here that looks useful.



Shortcuts How to Add

Workspace



Name

- data
- exactmass
- filenames
- ndatass
- nommass
- ntestdatass
- samplenames
- testdata
- testfiles
- testsamples
- totalcounts

Current Directory Workspace

Command History

---%-- 10/8/10 10:49

Data Selection Panel

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Name of Data Matrix: Name of Variable Matrix: Name of Filename Matrix: Name of Totalcounts Matrix: Name of Samplenames Matrix:

Input Information

Make sure the data selected above is the data you want to analyze and then press the "Load Selected Data" button.

Load Selected Data

Data: **ndatass**
 Samples: **samplenames**
 Variables: **exactmass**

Scaling Method

Mean Center

Run PCA

Show Eigenvalue Scree Plot

PCA Summary

PC#	%Var	%Vartotal
1	52.3	52.3
2	20.6	73
3	13.7	86.7
4	7.1	93.8
5	3.5	97.2
6	1.5	98.8
7	1	99.7
8	0.1	99.8
9	0.1	99.9
10	0	99.9

PCA Panel

Plot PCA Scores and Loadings

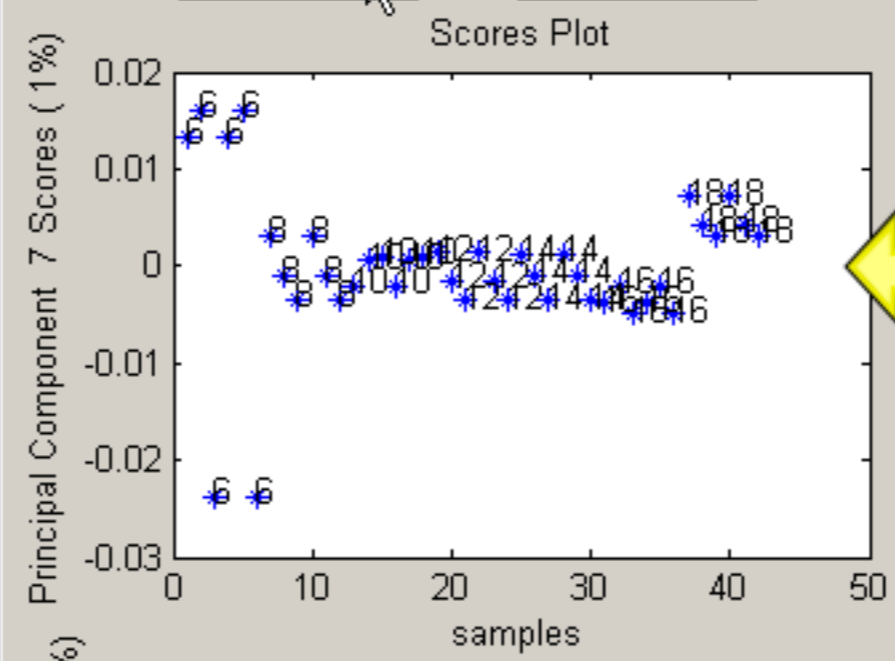
These plots are for a quick check of the results and cannot be saved.

Loading plots default to m/z vs PC#.

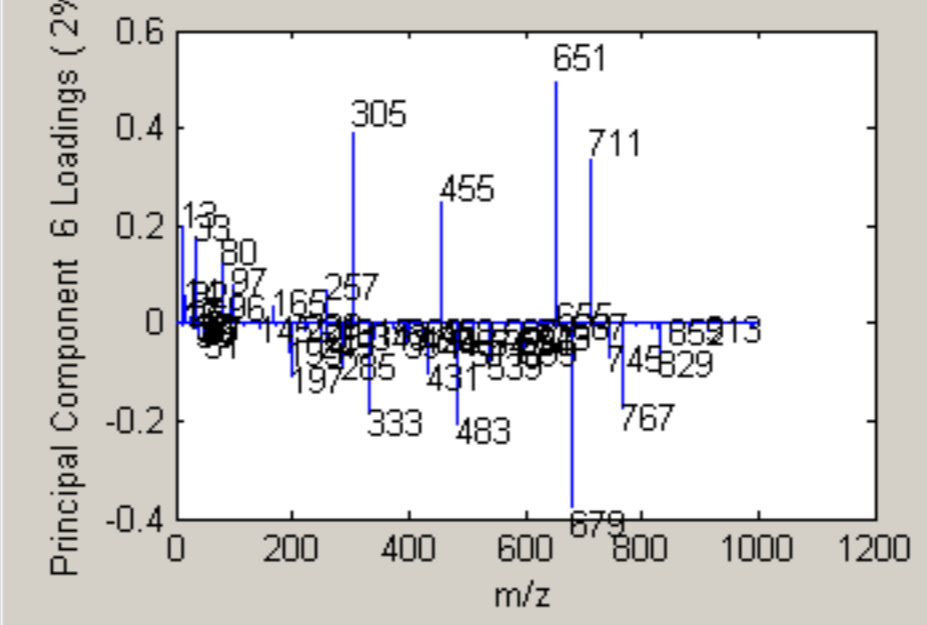
samp/var 7

Plot Scores

Plot Loads



PC7 looks like it is capturing some scatter in sample 6, and maybe something in sample 18.



Save PCA Data to Workspace

Number of PCs to keep

Input field for number of PCs to keep

Scores output name

Input field for scores output name

Loadings output name

Input field for loadings output name

Save To Workspace

Close Panel

Workspace

- data
- exactmass
- filenames
- ndatass
- nommass
- ntestdatass
- samplenames
- testdata
- testfiles
- testsamples
- totalcounts

Current Directory Workspace

Command History

---%-- 10/8/10 10:49

Data Selection Panel

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Name of Data Matrix: Name of Variable Matrix: Name of Filename Matrix: Name of Totalcounts Matrix: Name of Samplenames Matrix:

Input Information

Make sure the data selected above is the data you want to analyze and then press the "Load Selected Data" button.

Load Selected Data

Data: **ndatass**
 Samples: **samplenames**
 Variables: **exactmass**

Scaling Method

Run PCA

Show Eigenvalue Scree Plot

PCA Summary

PC#	%Var	%Vartotal
1	52.3	52.3
2	20.6	73
3	13.7	86.7
4	7.1	93.8
5	3.5	97.2
6	1.5	98.8
7	1	99.7
8	0.1	99.8
9	0.1	99.9
10	0	99.9

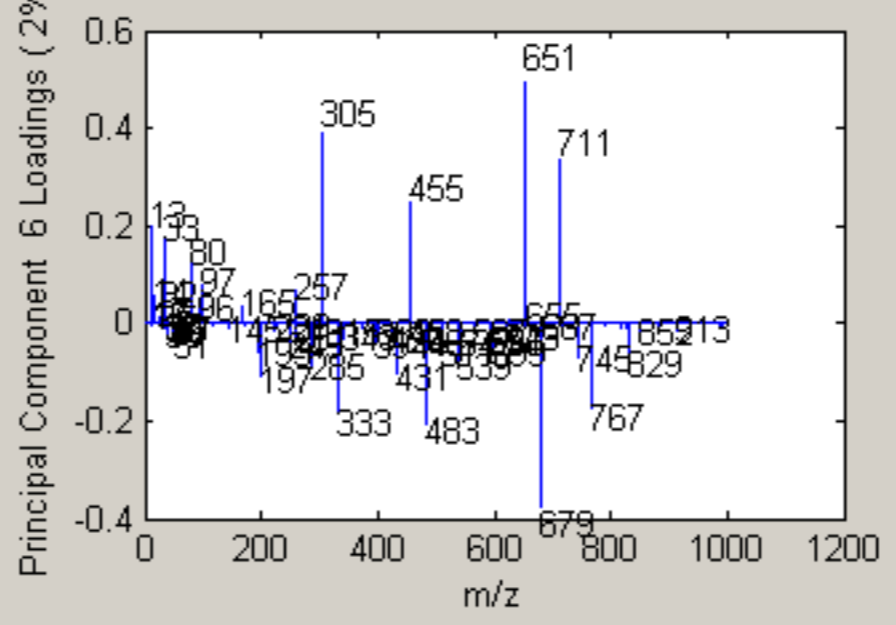
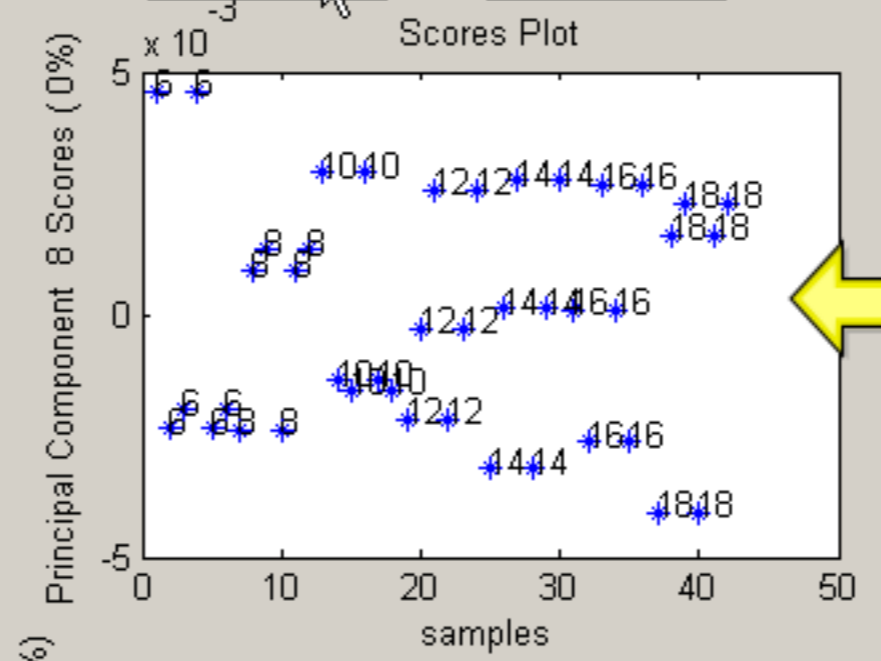
PCA Panel

Plot PCA Scores and Loadings

These plots are for a quick check of the results and cannot be saved.

Loading plots default to m/z vs PC#.

samp/var:



Save PCA Data to Workspace

Number of PCs to keep:

Scores output name:

Loadings output name:

PC8 definitely looks like it is mainly noise in the data.

Save To Workspace

Close Panel

Workspace

- data
- exactmass
- filenames
- ndatass
- nommass
- ntestdatass
- samplenames
- testdata
- testfiles
- testsamples
- totalcounts

Current Directory Workspace

Command History

---%-- 10/8/10 10:49

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Name of Data Matrix: Name of Variable Matrix: Name of Filename Matrix: Name of Totalcounts Matrix: Name of Samplenames Matrix:

Input Information

Make sure the data selected above is the data you want to analyze and then press the "Load Selected Data" button.

Load Selected Data

Data: **ndatass**
 Samples: **samplenames**
 Variables: **exactmass**

Scaling Method:

Run PCA

Show Eigenvalue Scree Plot

PCA Summary

PC#	%Var	%Vartotal
1	52.3	52.3
2	20.6	73
3	13.7	86.7
4	7.1	93.8
5	3.5	97.2
6	1.5	98.8
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8	0.1	99.8
9	0.1	99.9
10	0	99.9

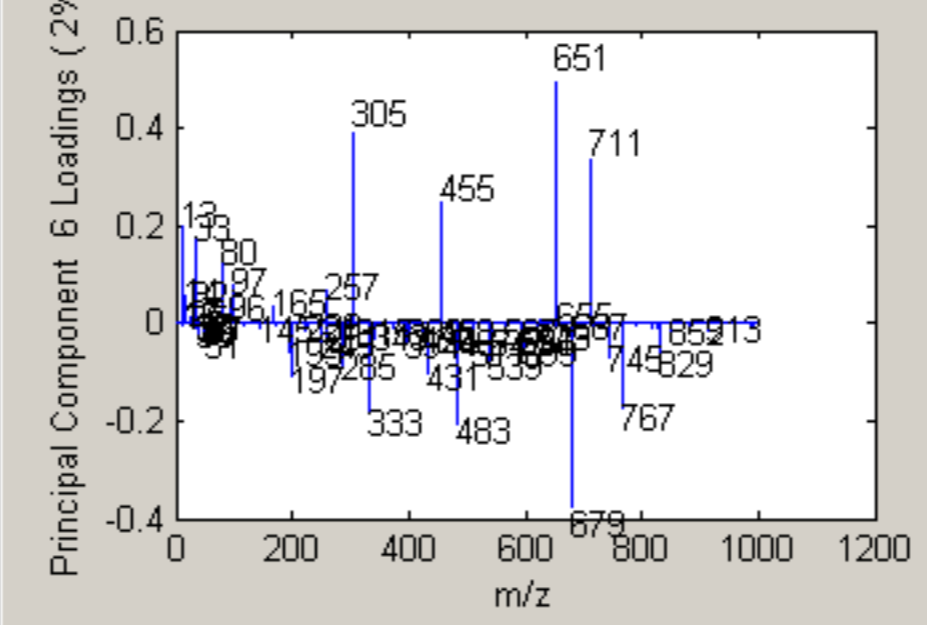
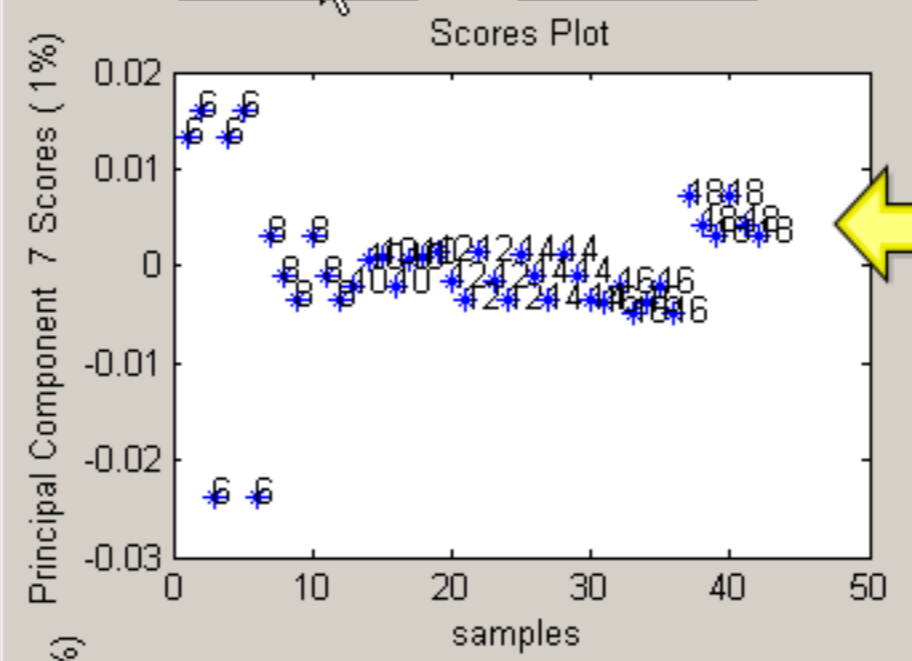
PCA Panel

Plot PCA Scores and Loadings

These plots are for a quick check of the results and cannot be saved.

Loading plots default to m/z vs PC#.

samp/var:
Plot Scores **Plot Loads**



Save PCA Data to Workspace

Number of PCs to keep:

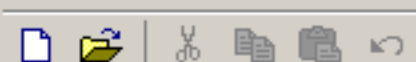
Scores output name:

Loadings output name:

Save To Workspace

Close Panel

Note how PC8 showed scatter while there is at least some pattern in PC7.



Shortcuts [How to Add](#)

Workspace

Name
data
exactmass
filenames
ndatass
nommass
ntestdatass
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testdata
testfiles
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totalcounts

Current Directory Workspace

Command History

```

>> 10/8/10 10:49
    
```

Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise. Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix <input type="text" value="ndatass"/>	Name of Variable Matrix <input type="text" value="exactmass"/>	Name of Filename Matrix <input type="text" value="filenames"/>	Name of Totalcounts Matrix <input type="text" value="totalcounts"/>	Name of Samplenames Matrix <input type="text" value="samplenames"/>
---	---	---	--	--

Input Information

Make sure the data selected above is the data you want to analyze and then press the "Load Selected Data" button.

Load Selected Data

Data: **ndatass**
 Samples: **samplenames**
 Variables: **exactmass**

Scaling Method

Run PCA

Show Eigenvalue Scree Plot

PCA Summary

PC#	%Var	%Vartotal
1	52.3	52.3
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10	0	99.9

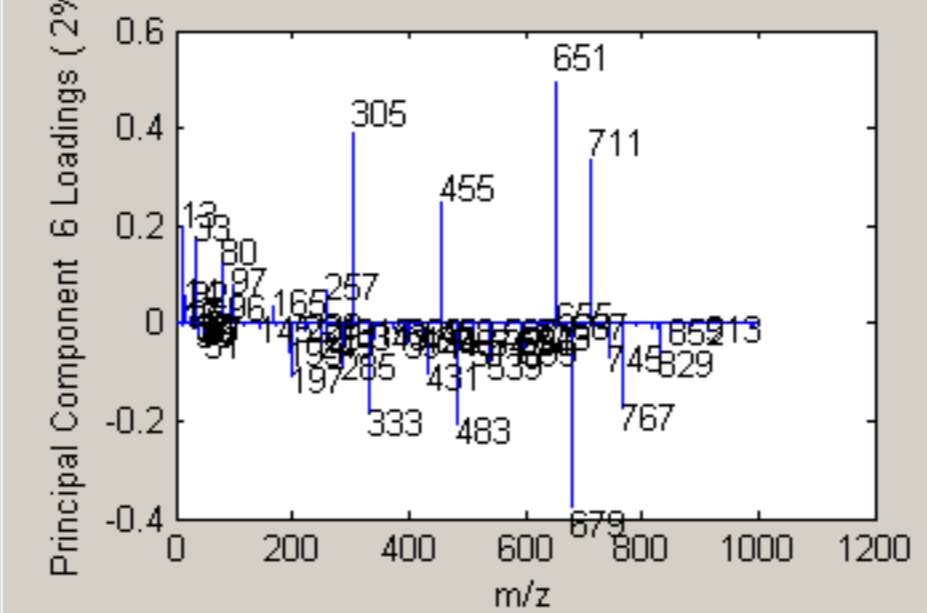
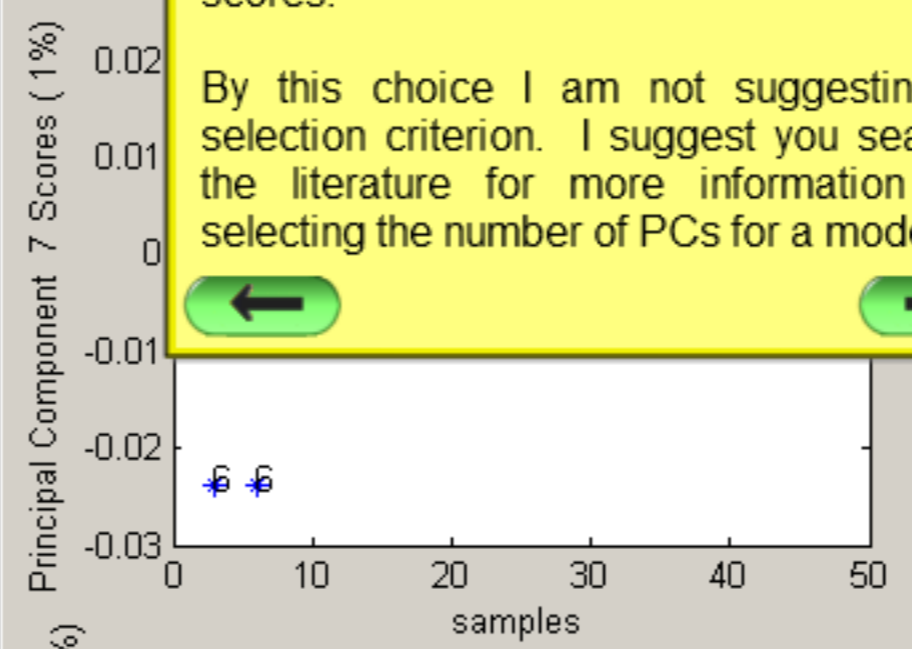
PCA Panel

Plot PCA Scores and Loadings

These plots are for a quick check of the results and cannot be saved.

While there may be some question about whether to keep 6 or 7 PCs for this model, for the sake of this tutorial we will keep all PCs up to where there is just noise in the scores.

By this choice I am not suggesting a selection criterion. I suggest you search the literature for more information on selecting the number of PCs for a model.



Save PCA Data to Workspace

Number of PCs to keep

Scores output name

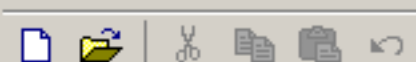
Loadings output name

Percent variance output name

Model output name

Save To Workspace

Close Panel



Shortcuts How to Add

Workspace

Name
data
exactmass
filenames
ndatass
nommass
ntestdatass
samplenames
testdata
testfiles
testsamples
totalcounts

Current Directory Workspace

Command History

---%-- 10/8/10 10:49

Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise. Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix <input type="text" value="ndatass"/>	Name of Variable Matrix <input type="text" value="exactmass"/>	Name of Filename Matrix <input type="text" value="filenames"/>	Name of Totalcounts Matrix <input type="text" value="totalcounts"/>	Name of Samplenames Matrix <input type="text" value="samplenames"/>
---	---	---	--	--

Input Information

Make sure the data selected above is the data you want to analyze and then press the "Load Selected Data" button.

Load Selected Data

Data: **ndatass**
 Samples: **samplenames**
 Variables: **exactmass**

Scaling Method

Run PCA

Show Eigenvalue Scree Plot

PCA Summary

PC#	%Var	%Vartotal
1	52.3	52.3
2	20.6	73
3	13.7	86.7
4	7.1	93.8
5	3.5	97.2
6	1.5	98.8
7	1	99.7
8	0.1	99.8
9	0.1	99.9
10	0	99.9

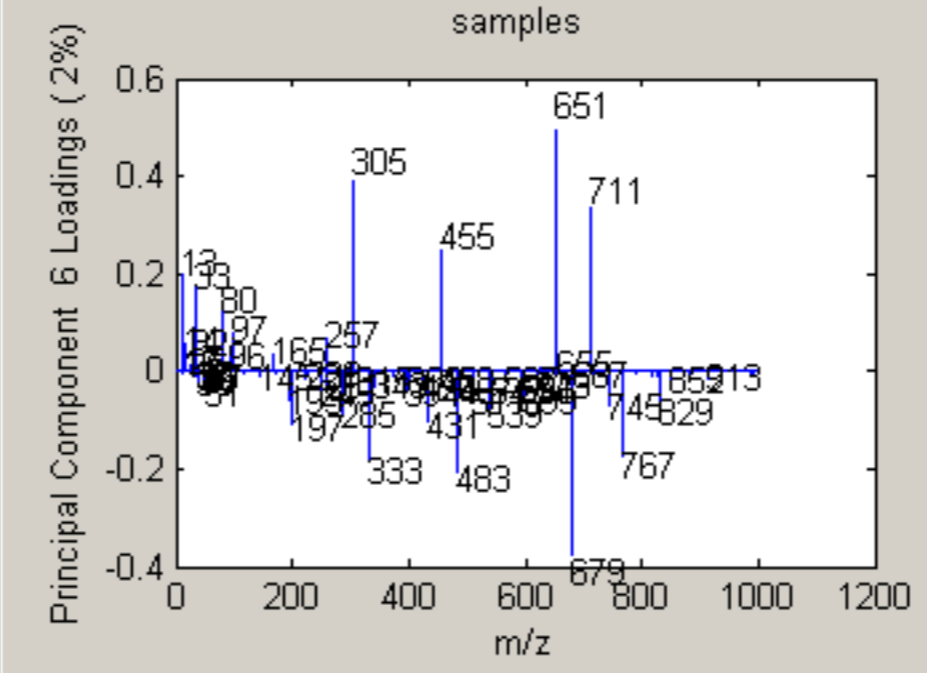
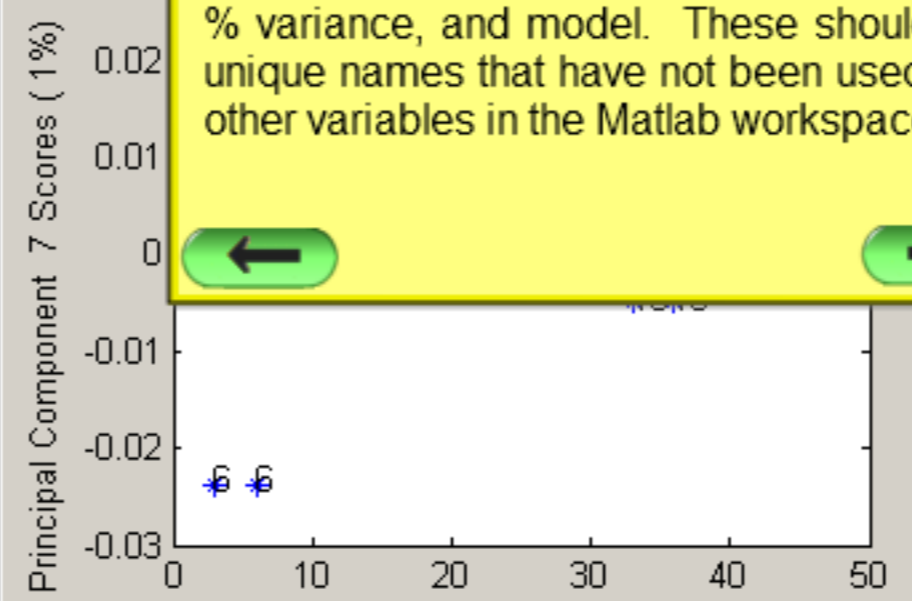
PCA Panel

Plot PCA Scores and Loadings

These plots are for a quick check of the results and cannot be saved.

Loading plots default to m/z vs PC#.

Now enter names for the scores, loadings, % variance, and model. These should be unique names that have not been used for other variables in the Matlab workspace.



Save PCA Data to Workspace

Number of PCs to keep

Scores output name

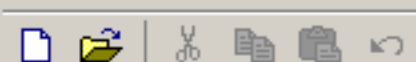
Loadings output name

Percent variance output name

Model output name

Save To Workspace

Close Panel



Shortcuts How to Add

Workspace

Name
data
exactmass
filenames
ndatass
nommass
ntestdatass
samplenames
testdata
testfiles
testsamples
totalcounts

Current Directory Workspace

Command History

---%-- 10/8/10 10:49

Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise. Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix <input type="text" value="ndatass"/>	Name of Variable Matrix <input type="text" value="exactmass"/>	Name of Filename Matrix <input type="text" value="filenames"/>	Name of Totalcounts Matrix <input type="text" value="totalcounts"/>	Name of Samplenames Matrix <input type="text" value="samplenames"/>
---	---	---	--	--

Input Information

Make sure the data selected above is the data you want to analyze and then press the "Load Selected Data" button.

Load Selected Data

Data: **ndatass**
 Samples: **samplenames**
 Variables: **exactmass**

Scaling Method

Run PCA

Show Eigenvalue Scree Plot

PCA Summary

PC#	%Var	%Vartotal
1	52.3	52.3
2	20.6	73
3	13.7	86.7
4	7.1	93.8
5	3.5	97.2
6	1.5	98.8
7	1	99.7
8	0.1	99.8
9	0.1	99.9
10	0	99.9

PCA Panel

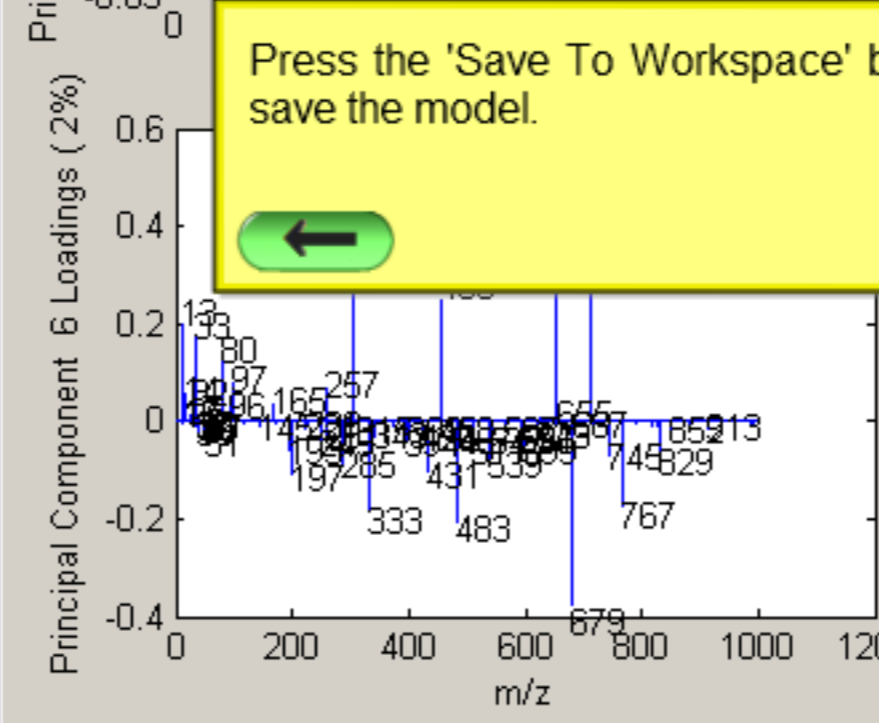
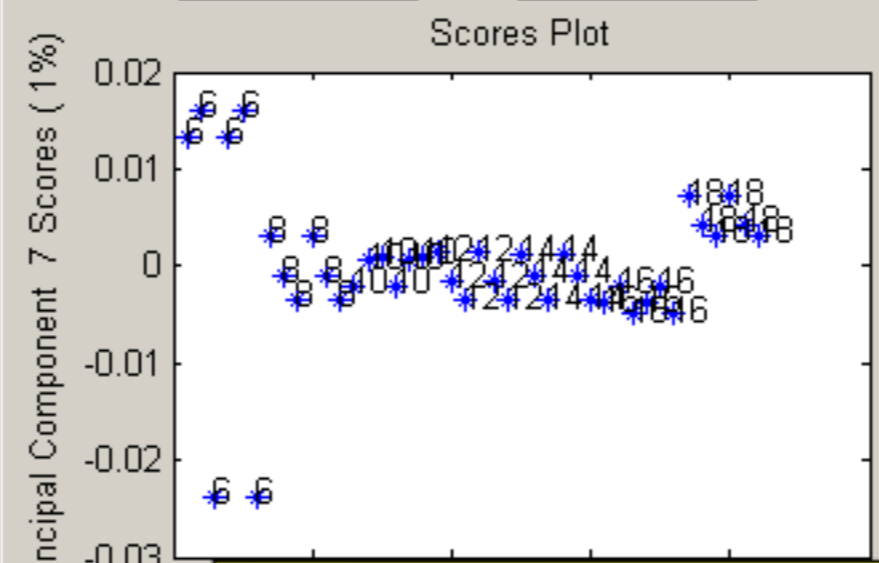
Plot PCA Scores and Loadings

These plots are for a quick check of the results and cannot be saved.

Loading plots default to m/z vs PC#.

samp/var

Plot Scores Plot Loads



Press the 'Save To Workspace' button to save the model.



Save PCA Data to Workspace

Number of PCs to keep

 Scores output name

Loadings output name

Percent variance output name

Model output name

Save To Workspace

Close Panel



Workspace



Name

- data
- exactmass
- filenames
- ndatass
- nommass
- ntestdatass
- pca loads
- pcamodel
- pcascores
- pcavariance
- samplenames
- testdata
- testfiles
- testsamples
- totalcounts

Current Directory Workspace

Command History

---%-- 10/8/10 10:49

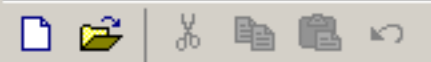
Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise. Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix	Name of Variable Matrix	Name of Filename Matrix	Name of Totalcounts Matrix	Name of Samplenames Matrix
ndatass	exactmass	filenames	totalcounts	samplenames

Now we will use the model we just created and project new data into it.

← →



Workspace

- Name
- data
- exactmass
- filenames
- ndatass
- nommass
- ntestdatass
- pca loads
- pcamodel
- pcascores
- pcavariance
- samplenames
- testdata
- testfiles
- testsamples
- totalcounts

Command History

```
---%-- 10/8/10 10:49
```

- Run PCA
- PCA Modelling
- Run DPCA
- Export MVA Data

From the 'MVA' menu choose -> 'PCA Modelling'

Name of Data Matrix
ndatass

Name of Vari
exactmass

menames

of Totalcounts Matrix
totalcounts

Name of Samplenames Matrix
samplenames



Shortcuts How to Add

Workspace

- Name
- data
- exactmass
- filenames
- ndatass
- nommass
- ntestdatass
- pcalloads
- pcamodel
- pcascores
- pcavarience
- samplenames
- testdata
- testfiles
- testsamples
- totalcounts

Current Directory Workspace

Command History

---%-- 10/8/10 10:49

Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise. Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix: **ndatass** | Name of Variable Matrix: **exactmass** | Name of Filename Matrix: **filenames** | Name of Totalcounts Matrix: **totalcounts** | Name of Samplenames Matrix: **samplenames**

PCA Modelling Panel

Choose a Model to Load

Select Model

Select the data you want to project

Select the model we just created from this drop down menu.

Save Model Data to Workspace

Model Information	
Original Data Set	
Data:	None
Variables:	None
Samples:	None
Model Data	
Scores:	None
Loads:	None
% Variance:	None
Scaling Choice:	None

← →

New Data: None
New Samplenames: None

Name for New Data Scores

Save New Scores

Name for combined scores (new and model)

Save Combined Scores

Project Data Into Model

Close Panel



Shortcuts How to Add

Workspace



- Name
- data
- exactmass
- filenames
- ndatass
- nommass
- ntestdatass
- pcalloads
- pcamodel
- pcascores
- pcavarience
- samplenames
- testdata
- testfiles
- testsamples
- totalcounts

Current Directory Workspace

Command History

---%-- 10/8/10 10:49

Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise. Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix: Name of Variable Matrix: Name of Filename Matrix: Name of Totalcounts Matrix: Name of Samplenames Matrix:

PCA Modelling Panel

Choose a Model to Load

Select the data you want to project into the model, and corresponding samplenames from the 'Raw Data Selection Panel'

Save Model Data to Workspace

Model Information	
Original Data Set	
Data:	ndatass
Variables:	exactmass
Samples:	samplenames
Model Data	
Scores:	pcascores
Loads:	pcalloads
% Variance:	pcavarience
Scaling Choice:	Mean Center

The model keeps a reference to what data was used to create the model. That way you can remember exactly what data was used so you can go back and adjust the model if you need to.

This information is listed here in the 'Original Data Set' box.

Name for New Data Scores

Save New Scores

combined (with model)

Save Combined Scores

Close Panel



Shortcuts How to Add

Workspace

- Name
- data
- exactmass
- filenames
- ndatass
- nommass
- ntestdatass
- pcalloads
- pcamodel
- pcascores
- pcavarience
- samplenames
- testdata
- testfiles
- testsamples
- totalcounts

Current Directory Workspace

Command History

---%-- 10/8/10 10:49

Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise. Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix: Name of Variable Matrix: Name of Filename Matrix: Name of Totalcounts Matrix: Name of Samplenames Matrix:

PCA Modelling Panel

Choose a Model to Load

Select the data you want to project into the model, and corresponding samplenames from the 'Raw Data Selection Panel'

New Data: New Samplenames:

Save Model Data to Workspace

Name for New Data Scores

Name for combined scores (new and model)

Model Information

Original Data Set

Data: **ndatass**
 Variables: **exactmass**
 Samples: **samplenames**

Model Data

Scores: **pcascores**
 Loads: **pcalloads**
 % Variance: **pcavarience**
 Scaling Choice: **Mean Center**

The 'Model Data' box lists the names of the PCA results that are stored in the model and the scaling/pre-processing methods used in the model.

Workspace

Name ▲

- data
- exactmass
- filenames
- ndatass
- nommass
- ntestdatass
- pca loads
- pcamodel
- pcascores
- pcavariance
- samplenames
- testdata
- testfiles
- testsamples
- totalcounts

Current Directory Workspace

Command History

```

>> 10/8/10 10:49

```

Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise. Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix:

Name of Variable Matrix:

Name of Filename Matrix:

Name of Totalcounts Matrix:

Name of Samplenames Matrix:

PIA Modelling Panel

After loading the model, select the new data that you want to project into the model from the 'Data Selection Panel'.

You need to select the data and samplenames. Here I also select the filenames though they are not required for the function.

← →

Samples: **samplenames**

Model Data

Scores: **pcascores**

Loads: **pca loads**

% Variance: **pcavariance**

Scaling Choice: **Mean Center**

data you want to project into the model, and corresponding samplenames from the 'Data Selection Panel'

Selected Data

New Data: **None**

New Samplenames: **None**

Project Data Into Model

Save Model Data to Workspace

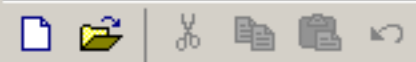
Name for New Data Scores:

Save New Scores

Name for combined scores (new and model):

Save Combined Scores

Close Panel



Shortcuts How to Add

Workspace



Name

- data
- exactmass
- filenames
- ndatass
- nommass
- ntestdatass
- pcalloads
- pcamodel
- pcascores
- pcavarience
- samplenames
- testdata
- testfiles
- testsamples
- totalcounts

Current Directory Workspace

Command History

---%-- 10/8/10 10:49

Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise. Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix:
 Name of Variable Matrix:
 Name of Filename Matrix:
 Name of Totalcounts Matrix:
 Name of Samplenames Matrix:

PCA Modelling Panel

Choose a Model to Load

Select the data you want to project into the model, and corresponding samplenames from the 'Raw Data Selection Panel'

Save Model Data to Workspace

Model Information

Original Data Set

Data: **ndatass**
 Variables: **exactmass**
 Samples: **samplenames**

Scores:
 Loads:
 % Variance:
 Scaling Cho

Load Selected Data

New Data:
 New Samplenames:

Name for New Data Scores

Save New Scores

Name for combined scores (new and model)

Save Combined Scores

Now load the new data into the panel using the 'Load Selected Data' button.

← →

Close Panel



Shortcuts How to Add

Workspace



Name

- data
- exactmass
- filenames
- ndatass
- nommass
- ntestdatass
- pcalloads
- pcamodel
- pcascores
- pcavarience
- samplenames
- testdata
- testfiles
- testsamples
- totalcounts

Current Directory Workspace

Command History

---%-- 10/8/10 10:49

Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise. Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix	Name of Variable Matrix	Name of Filename Matrix	Name of Totalcounts Matrix	Name of Samplenames Matrix
<input type="text" value="ntestdatass"/>	<input type="text" value="exactmass"/>	<input type="text" value="testfiles"/>	<input type="text" value="totalcounts"/>	<input type="text" value="testsamples"/>

PCA Modelling Panel

Choose a Model to Load

Model Information	
Original Data Set	
Data:	ndatass
Variables:	exactmass
Samples:	samplenames
Model Data	
Scores:	pcascores
Loads:	pcalloads
% Variance:	pcavarience
Scaling Choice:	Mean Center

Select the data you want to project into the model, and corresponding samplenames from the 'Raw Data Selection Panel'

New Data:	ntestdatass
New Samplenames:	testsamples

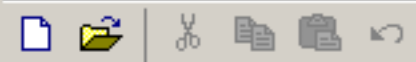
Use this button to apply the model to the selected data

Save Model Data to Workspace

Name for New Data Scores

Name for combined scores (new and model)

Press the 'Project Data Into Model' to projec the new data into the PCA model.



Workspace

- Name
- data
- exactmass
- filenames
- ndatass
- nommass
- ntestdatass
- pcalloads
- pcamodel
- pcascores
- pcavariance
- samplenames
- sgnewx
- testdata
- testfiles
- testsamples
- totalcounts

Current Directory Workspace

Command History

---%-- 10/8/10 10:49

Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise. Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix: Name of Variable Matrix: Name of Filename Matrix: Name of Totalcounts Matrix: Name of Samplenames Matrix:

PCA Modelling Panel

Choose a Model to Load

Model Information

Original Data Set

Data: **ndatass**
 Variables: **exactmass**
 Samples: **samplenames**

Model Data

Scores: **pcascores**
 Loads: **pcalloads**
 % Variance: **pcavariance**
 Scaling Choice: **Mean Center**

Select the data you want to project into the model, and corresponding samplenames from the 'Raw Data Selection Panel'

New Data: **ntestdatass**
 New Samplenames: **testsamples**

Save Model Data to Workspace

Name for New Data Scores

Name for combined scores (new and model)

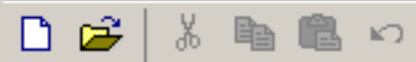
X-Axis: Y-Axis:

← This brings up a new panel where you can plot the new scores alone or combined with the model scores.

The loadings are not shown in this panel since they are the same as the model loadings and can be explored using the 'Plot Loadings' function in the 'Data Display' menu.

→

Panel



Shortcuts How to Add

Workspace

- Name
- data
- exactmass
- filenames
- ndatass
- nommass
- ntestdatass
- pcalloads
- pcamodel
- pcascores
- pcavariance
- samplenames
- sgnewx
- testdata
- testfiles
- testsamples
- totalcounts

Current Directory Workspace

Command History

---%-- 10/8/10 10:49

Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise. Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix: Name of Variable Matrix: Name of Filename Matrix: Name of Totalcounts Matrix: Name of Samplenames Matrix:

PCA Modelling Panel

Choose a Model to Load

Select the data you want to project into the model, and corresponding samplenames from the 'Raw Data Selection Panel'

Save Model Data to Workspace

Name for New Data Scores

Name for combined scores (new and model)

Model Information

Original Data Set

Data: **ndatass**
 Variables: **exactmass**
 Samples: **samplenames**

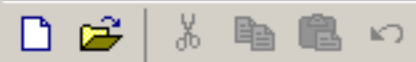
Model Data

Scores: **pcascores**
 Loads: **pcalloads**
 % Variance: **pcavariance**
 Scaling Choice: **Mean Center**

New Data: **ntestdatass**
 New Samplenames: **testsamples**

X-Axis:
 Y-Axis:

Let's look at the scores of the new data first.



Shortcuts How to Add

Workspace



Name

- data
- exactmass
- filenames
- ndatass
- nommass
- ntestdatass
- pcalloads
- pcamodel
- pcascores
- pcavariance
- samplenames
- sgnewx
- testdata
- testfiles
- testsamples
- totalcounts

Current Directory Workspace

Command History

---%-- 10/8/10 10:49

Command window area for MATLAB commands and output.

Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise. Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix: Name of Variable Matrix: Name of Filename Matrix: Name of Totalcounts Matrix: Name of Samplenames Matrix:

PCA Modelling Panel

Choose a Model to Load

Model Information

Original Data Set

Data: **ndatass**
 Variables: **exactmass**
 Samples: **samplenames**

Model Data

Scores: **pcascores**
 Loads: **pcalloads**
 % Variance: **pcavariance**
 Scaling Choice: **Mean Center**

Select the data you want to project into the model, and corresponding samplenames from the 'Raw Data Selection Panel'

New Data: **ntestdatass**
 New Samplenames: **testsamples**

Save Model Data to Workspace

Name for New Data Scores

Name for combined scores (new and model)

X-Axis: Y-Axis:

Press the 'Plot Scores - New Data' button to plot only the scores for the new data.

← →



Shortcuts How to Add

Workspace

- Name
- data
- exactmass
- filenames
- ndatass
- nommass
- ntestdatass
- pcalloads
- pcamodel
- pcascores
- pcavariance
- samplenames
- sgnewx
- testdata
- testfiles
- testsamples
- totalcounts

Current Directory Workspace

Command History

---%-- 10/8/10 10:49

Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise. Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix: Name of Variable Matrix: Name of Filename Matrix: Name of Totalcounts Matrix: Name of Samplenames Matrix:

PCA Modelling Panel

Choose a Model to Load

Model Information

Original Data Set

Data: **ndatass**
 Variables: **exactmass**
 Samples: **samplenames**

Model Data

Scores: **pcascores**
 Loads: **pcalloads**
 % Variance: **pcavariance**
 Scaling Choice: **Mean Center**

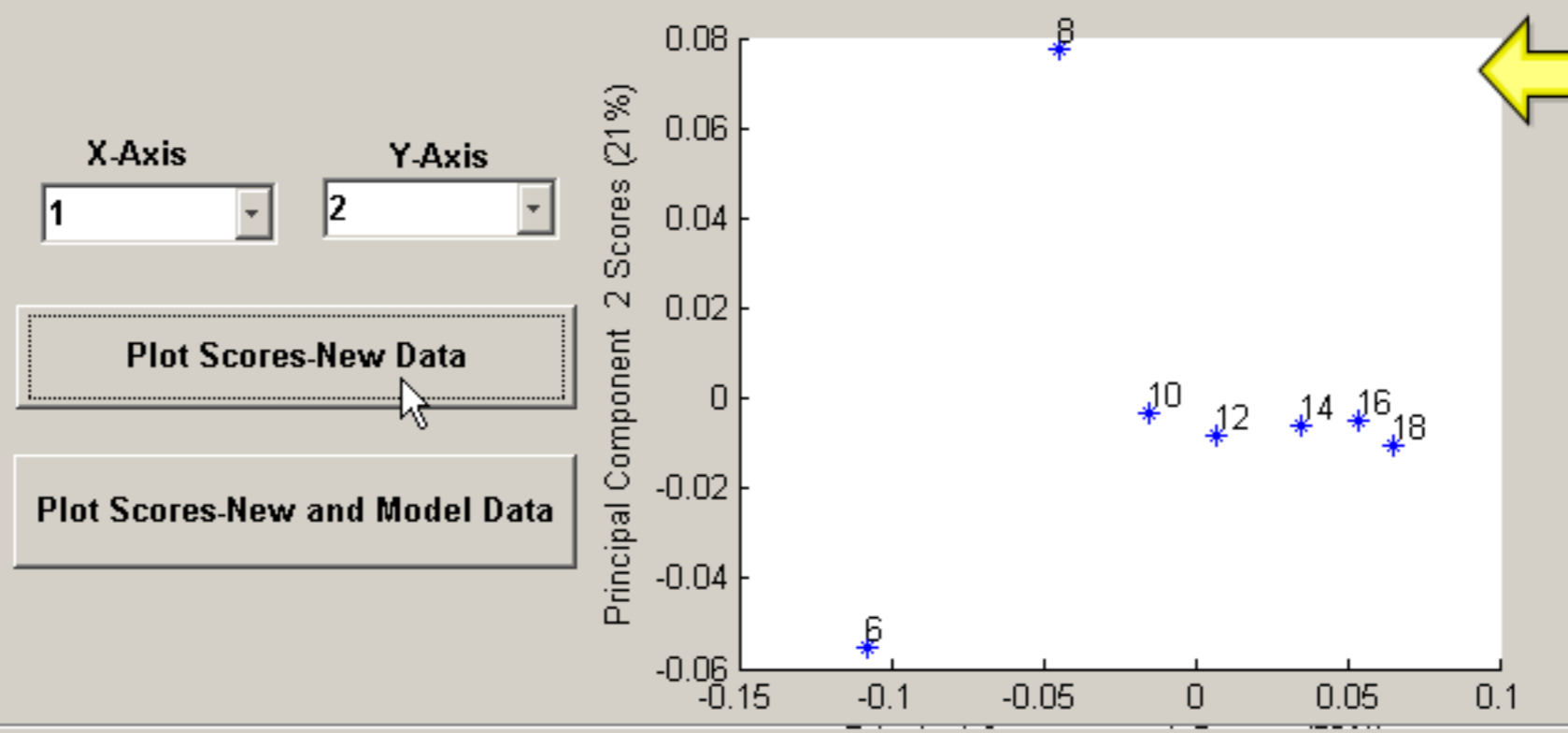
Select the data you want to project into the model, and corresponding samplenames from the 'Raw Data Selection Panel'

New Data: **ntestdatass**
 New Samplenames: **testsamples**

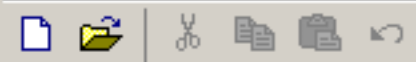
Save Model Data to Workspace

Name for New Data Scores

Name for combined scores (new and model)



Here we have plotted PC 1 vs PC2 scores for the new data.



Shortcuts How to Add

Workspace

- Name
- data
- exactmass
- filenames
- ndatass
- nommass
- ntestdatass
- pcalloads
- pcamodel
- pcascores
- pcavariance
- samplenames
- sgnewx
- testdata
- testfiles
- testsamples
- totalcounts

Current Directory Workspace

Command History

---%-- 10/8/10 10:49

Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise. Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix: Name of Variable Matrix: Name of Filename Matrix: Name of Totalcounts Matrix: Name of Samplenames Matrix:

PCA Modelling Panel

Choose a Model to Load

Model Information

Original Data Set

Data: **ndatass**
 Variables: **exactmass**
 Samples: **samplenames**

Model Data

Scores: **pcascores**
 Loads: **pcalloads**
 % Variance: **pcavariance**
 Scaling Choice: **Mean Center**

Select the data you want to project into the model, and corresponding samplenames from the 'Raw Data Selection Panel'

New Data: **ntestdatass**
 New Samplenames: **testsamples**

Save Model Data to Workspace

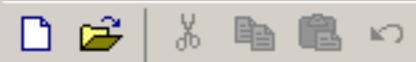
Name for New Data Scores

Name for combined scores (new and model)

X-Axis: Y-Axis:

Now lets look at all of the scores data together.

← →



Shortcuts How to Add

Workspace



Name

- data
- exactmass
- filenames
- ndatass
- nommass
- ntestdatass
- pcalloads
- pcamodel
- pcascores
- pcavariance
- samplenames
- sgnewx
- testdata
- testfiles
- testsamples
- totalcounts

Current Directory Workspace

Command History

10/8/10 10:49

Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise. Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix: Name of Variable Matrix: Name of Filename Matrix: Name of Totalcounts Matrix: Name of Samplenames Matrix:

PCA Modelling Panel

Choose a Model to Load

Model Information

Original Data Set

Data: **ndatass**
 Variables: **exactmass**
 Samples: **samplenames**

Model Data

Scores: **pcascores**
 Loads: **pcalloads**
 % Variance: **pcavariance**
 Scaling Choice: **Mean Center**

Select the data you want to project into the model, and corresponding samplenames from the 'Raw Data Selection Panel'

Load Selected Data

New Data: **ntestdatass**
 New Samplenames: **testsamples**

Project Data Into Model

Save Model Data to Workspace

Name for New Data Scores

Save New Scores

Name for combined scores (new and model)

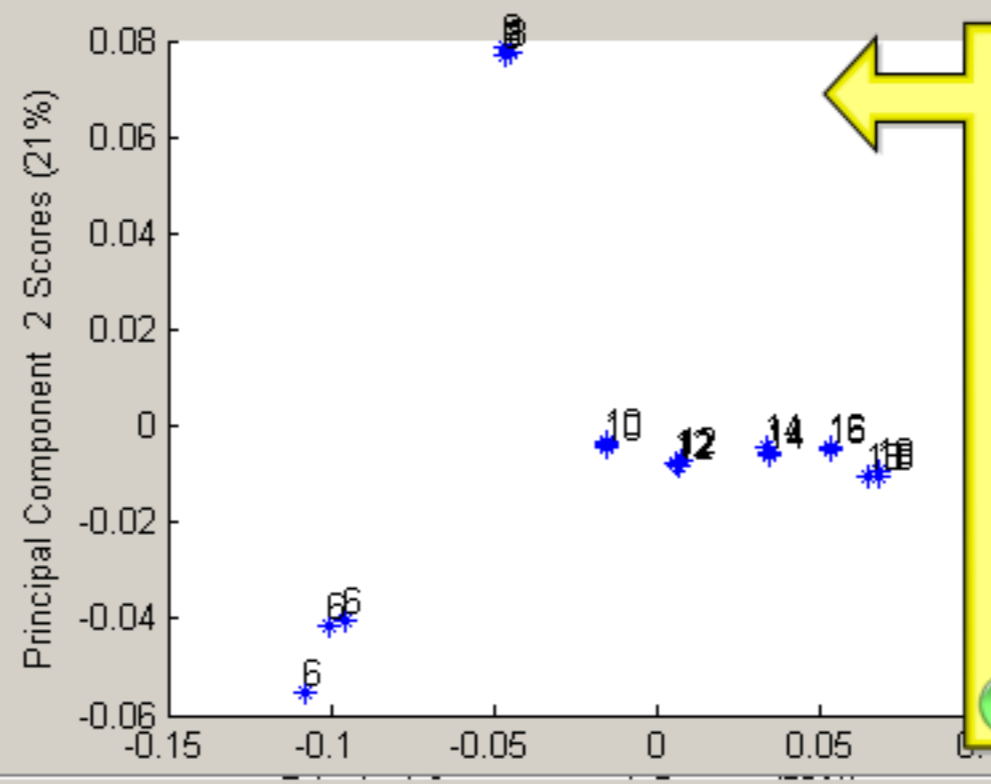
Save Combined Scores

X-Axis

Y-Axis

Plot Scores-New Data

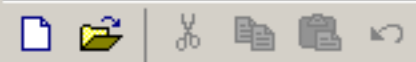
Plot Scores-New and Model Data



You can see that most new data points fall almost exactly where the model data points are.

At some point I may change the colors of the new scores and model scores to make them easier to see in the combined plot.

For now you can compare them by switching back and forth between the two plots.



Shortcuts How to Add

Workspace

- Name
- data
- exactmass
- filenames
- ndatass
- nommass
- ntestdatass
- pcalloads
- pcamodel
- pcascores
- pcavarience
- samplenames
- sgnewx
- testdata
- testfiles
- testsamples
- totalcounts

Current Directory Workspace

Command History

---%-- 10/8/10 10:49

Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise. Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix: Name of Variable Matrix: Name of Filename Matrix: Name of Totalcounts Matrix: Name of Samplenames Matrix:

PCA Modelling Panel

Choose a Model to Load

Select the data you want to project into the model, and corresponding samplenames from the 'Raw Data Selection Panel'

Save Model Data to Workspace

Name for New Data Scores

Name for combined scores (new and model)

Model Information

Original Data Set

Data: **ndatass**
 Variables: **exactmass**
 Samples: **samplenames**

Model Data

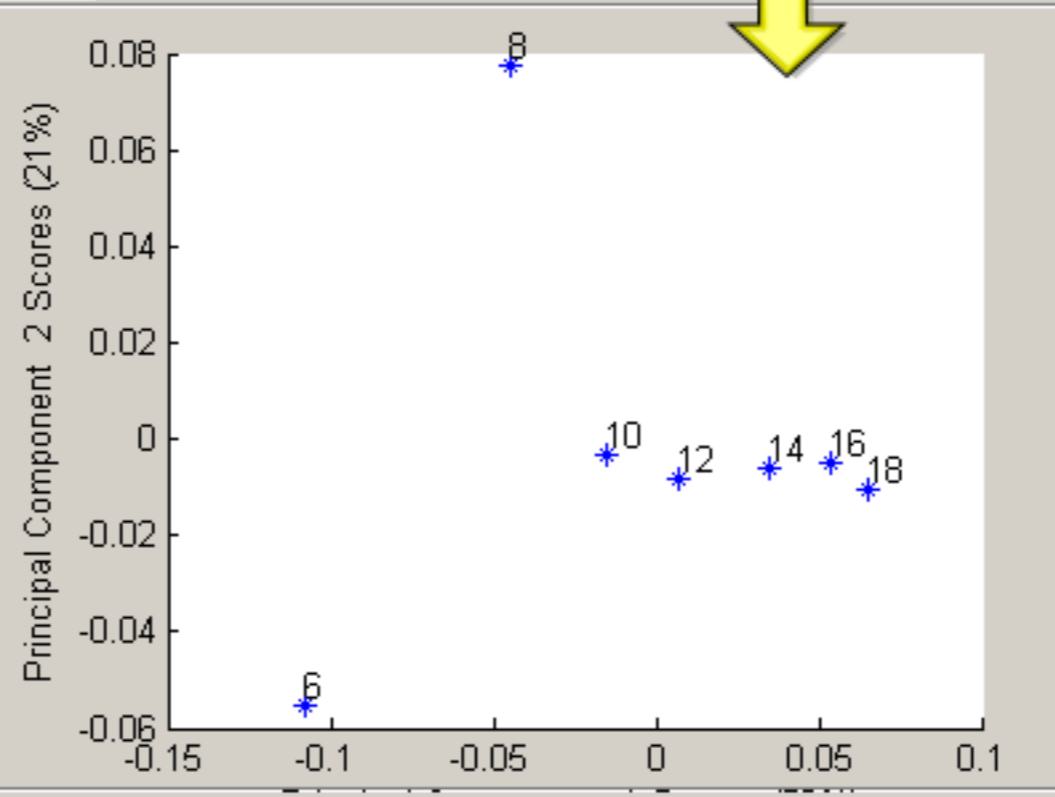
Scores: **pcas**
 Loads: **pcal**
 % Variance: **pcav**
 Scaling Choice: **Mean**

New Data: **ntestdatass**
 New Samplenames: **testsamples**

Just for reference. Here are the new sample scores alone.

← →

X-Axis: Y-Axis:





Shortcuts How to Add

Workspace

- Name
- data
- exactmass
- filenames
- ndatass
- nommass
- ntestdatass
- pcalloads
- pcamodel
- pcascores
- pcavariance
- samplenames
- sgnewx
- testdata
- testfiles
- testsamples
- totalcounts

Current Directory Workspace

Command History

---%-- 10/8/10 10:49

Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise. Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix: Name of Variable Matrix: Name of Filename Matrix: Name of Totalcounts Matrix: Name of Samplenames Matrix:

PCA Modelling Panel

Choose a Model to Load

Select the data you want to project into the model, and corresponding samplenames from the 'Raw Data Selection Panel'

Save Model Data to Workspace

Name for New Data Scores

Name for combined scores (new and model)

Model Information

Original Data Set

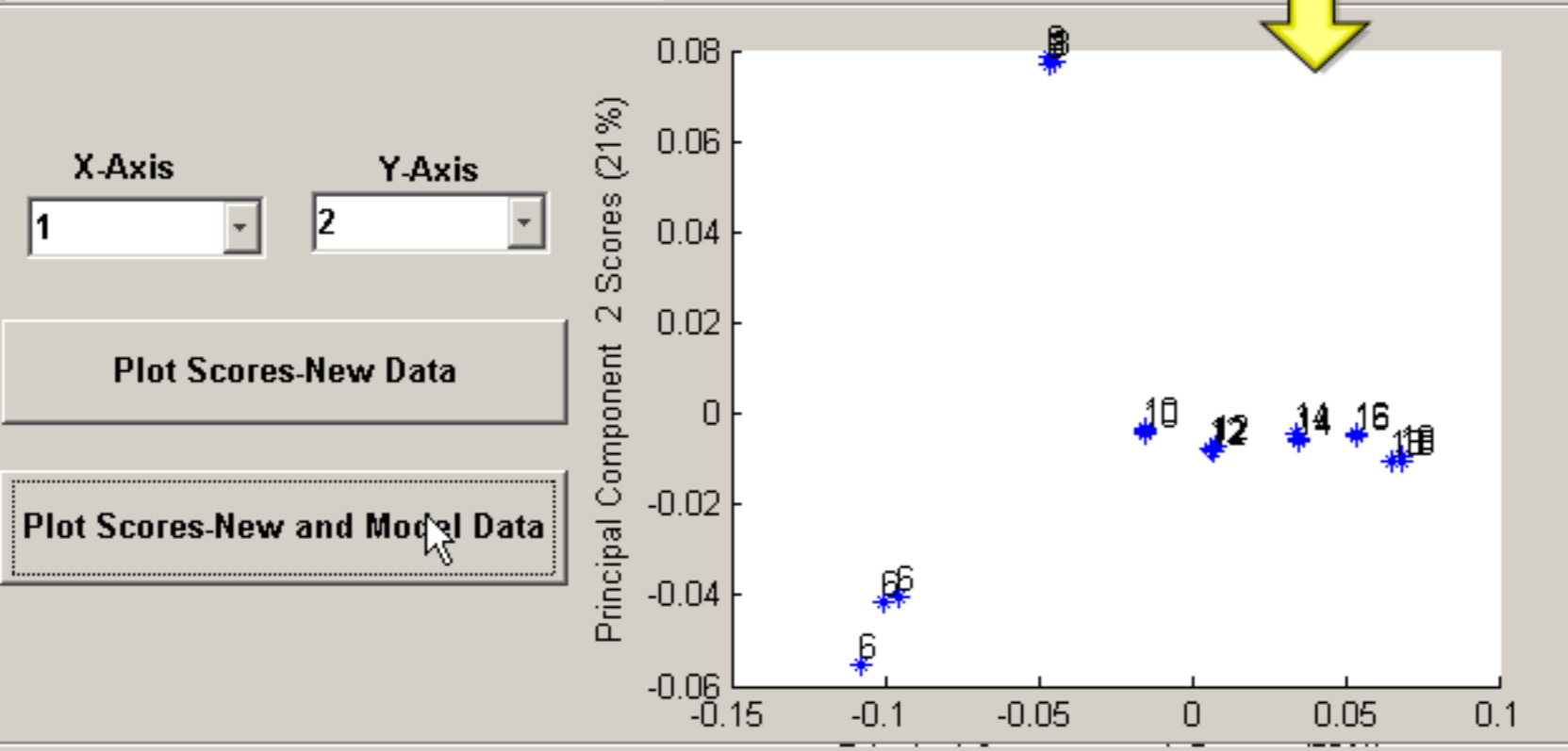
Data: **ndatass**
 Variables: **exactmass**
 Samples: **samplenames**

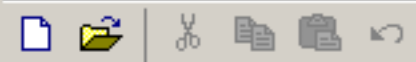
Model Data

Scores: **pcas**
 Loads: **pcal**
 % Variance: **pcav**
 Scaling Choice: **Mean**

New Data: **ntestdatass**
 New Samplenames: **testsamples**

And the combined scores again.





Shortcuts How to Add

Workspace

- Name
- data
- exactmass
- filenames
- ndatass
- nommass
- ntestdatass
- pcalloads
- pcamodel
- pcascores
- pcavariance
- samplenames
- sgnewx
- testdata
- testfiles
- testsamples
- totalcounts

Current Directory Workspace

Command History

---%-- 10/8/10 10:49

Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise. Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix: Name of Variable Matrix: Name of Filename Matrix: Name of Totalcounts Matrix: Name of Samplenames Matrix:

PCA Modelling Panel

Choose a Model to Load

Select the data you want to project into the model, and corresponding samplenames from the 'Raw Data Selection Panel'

Save Model Data to Workspace

Model Information

Original Data Set

Data: **ndatass**
 Variables: **exactmass**
 Samples: **samplenames**

Model Data

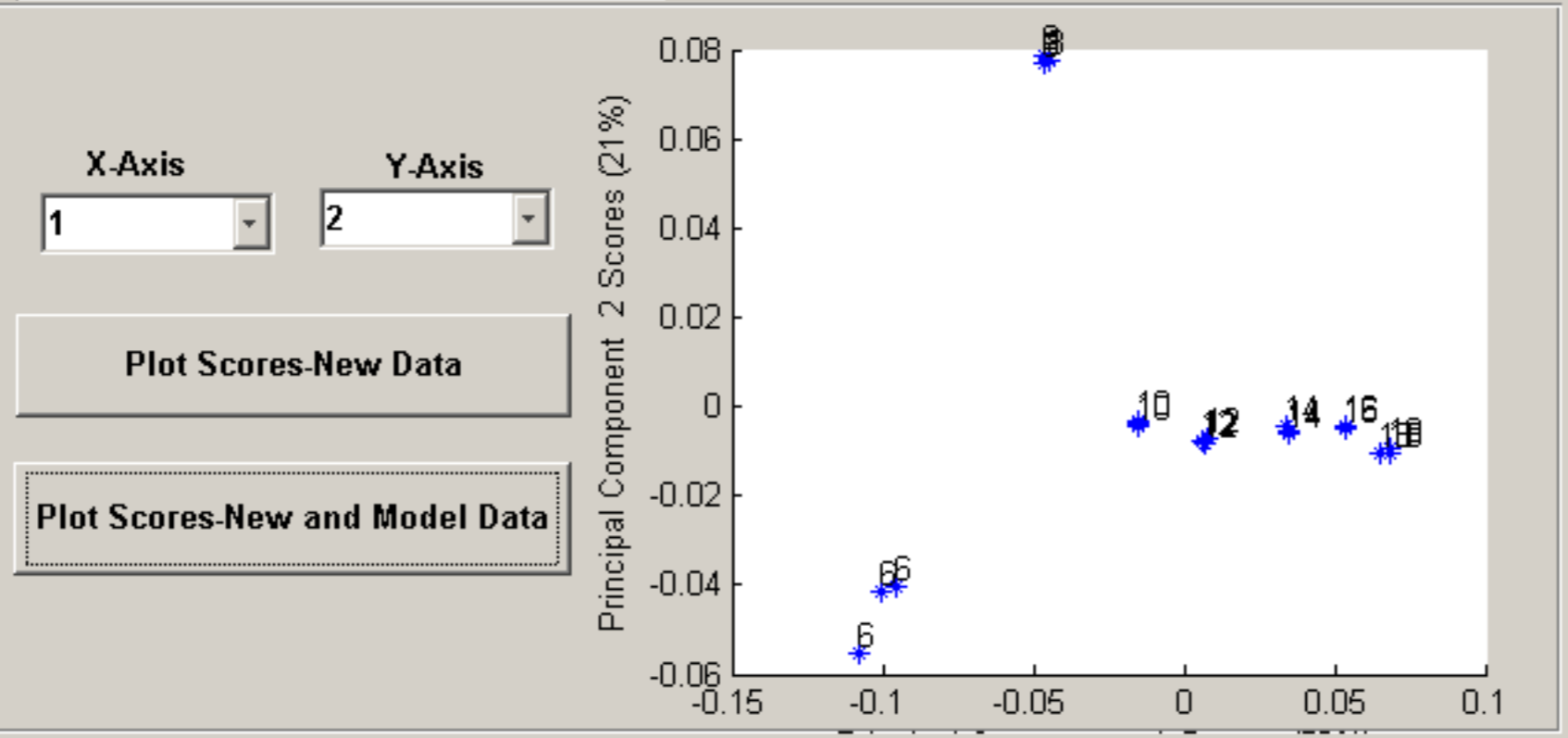
Scores: **pcascores**
 Loads: **pcalloads**
 % Variance: **pcavariance**
 Scaling Choice: **Mean Center**

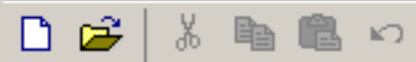
To save the scores for the new data only, enter a name for the new scores

← →

Name for New Data Scores:

Name for combined scores (new and model):





Shortcuts How to Add

Workspace

- Name
- data
- exactmass
- filenames
- ndatass
- nommass
- ntestdatass
- pcalloads
- pcamodel
- pcascores
- pcavariance
- samplenames
- sgnewx
- testdata
- testfiles
- testsamples
- totalcounts

Current Directory Workspace

Command History

---%-- 10/8/10 10:49

Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise. Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix: Name of Variable Matrix: Name of Filename Matrix: Name of Totalcounts Matrix: Name of Samplenames Matrix:

PCA Modelling Panel

Choose a Model to Load

Select the data you want to project into the model, and corresponding samplenames from the 'Raw Data Selection Panel'

Save Model Data to Workspace

Model Information

Original Data Set

Data: **ndatass**
 Variables: **exactmass**
 Samples: **samplenames**

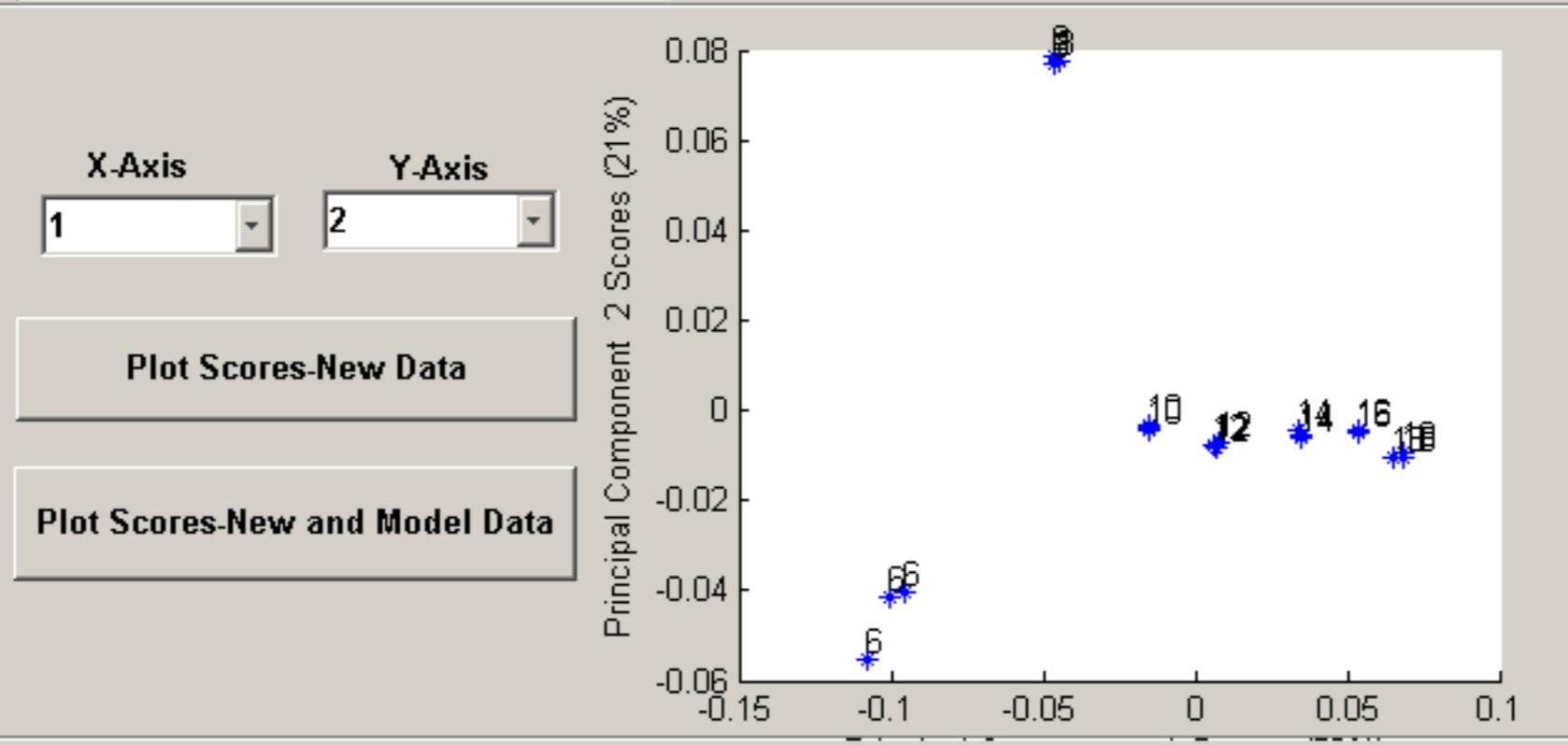
Model Data

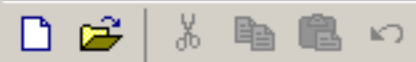
Scores: **pcascores**
 Loads: **pcalloads**
 % Variance: **pcavariance**
 Scaling Choice: **Mean Center**

and press the 'Save New Scores' button.

Name for New Data Scores:

Name for combined scores (new and model):





Shortcuts How to Add

Workspace

- Name
- data
- exactmass
- filenames
- ndatass
- newscores
- nommass
- ntestdatass
- pca loads
- pcamodel
- pcascores
- pcavariance
- samplenames
- sgnewx
- testdata
- testfiles
- testsamples
- totalcounts

Current Directory Workspace

Command History

---%-- 10/8/10 10:49

Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise. Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix: Name of Variable Matrix: Name of Filename Matrix: Name of Totalcounts Matrix: Name of Samplenames Matrix:

PCA Modelling Panel

Choose a Model to Load

Select the data you want to project into the model, and corresponding samplenames from the 'Raw Data Selection Panel'

Save Model Data to Workspace

Name for New Data Scores

Name for combined scores (new and model)

Model Information

Original Data Set

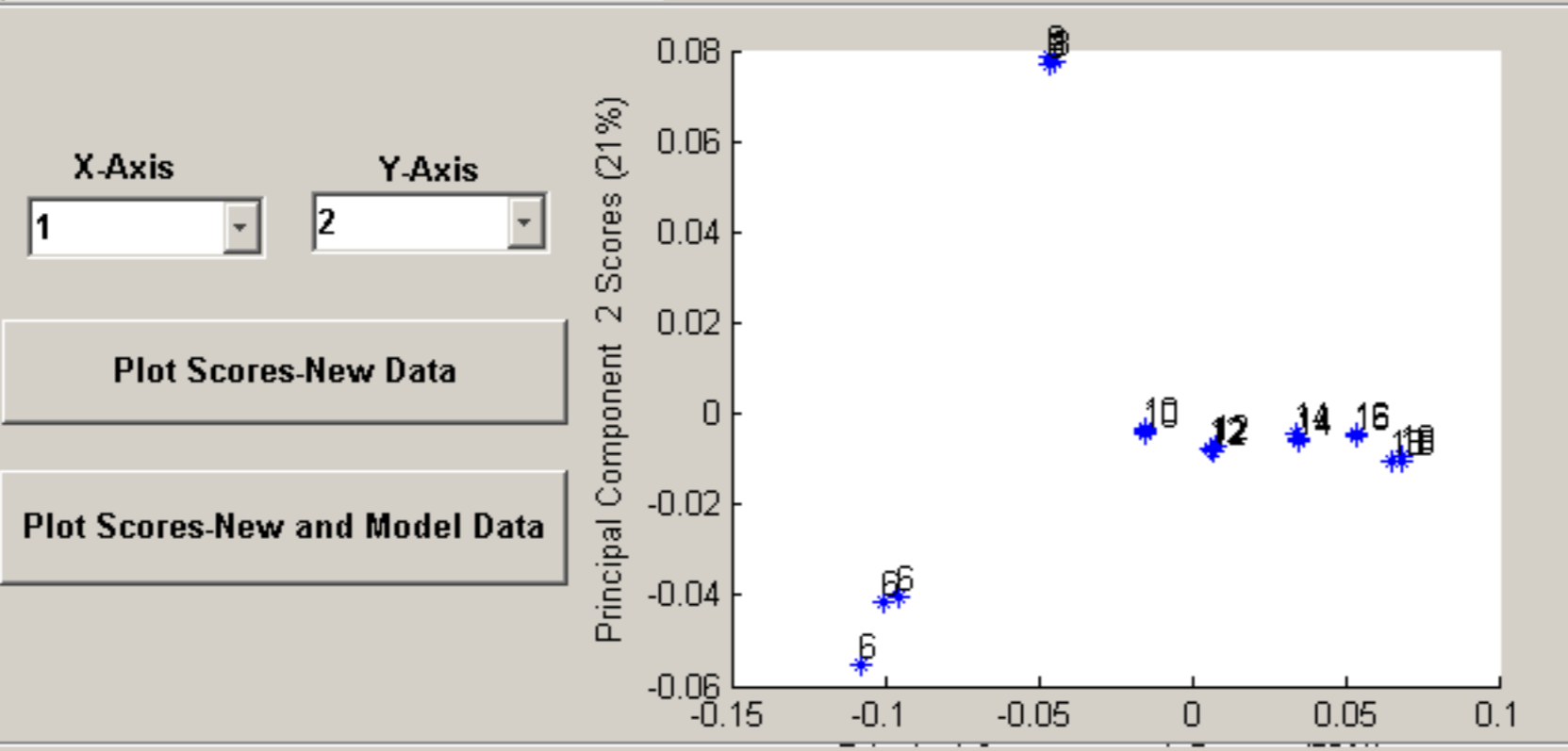
Data: **ndatass**
 Variables: **exactmass**
 Samples: **samplenames**

Model Data

Scores: **pcascores**
 Loads: **pca loads**
 % Variance: **pcavariance**
 Scaling Choice: **Mean Center**

New Data: **ntestdatass**

To save the combined scores enter a name for the combined scores





Shortcuts How to Add

Workspace

- Name
- data
- exactmass
- filenames
- ndatass
- newscores
- nommass
- ntestdatass
- pca loads
- pcamodel
- pcascores
- pcavariance
- samplenames
- sgnewx
- testdata
- testfiles
- testsamples
- totalcounts

Current Directory Workspace

Command History

---%-- 10/8/10 10:49

Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise. Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix: Name of Variable Matrix: Name of Filename Matrix: Name of Totalcounts Matrix: Name of Samplenames Matrix:

PCA Modelling Panel

Choose a Model to Load

Select the data you want to project into the model, and corresponding samplenames from the 'Raw Data Selection Panel'

Save Model Data to Workspace

Name for New Data Scores

Name for combined scores (new and model)

Model Information

Original Data Set

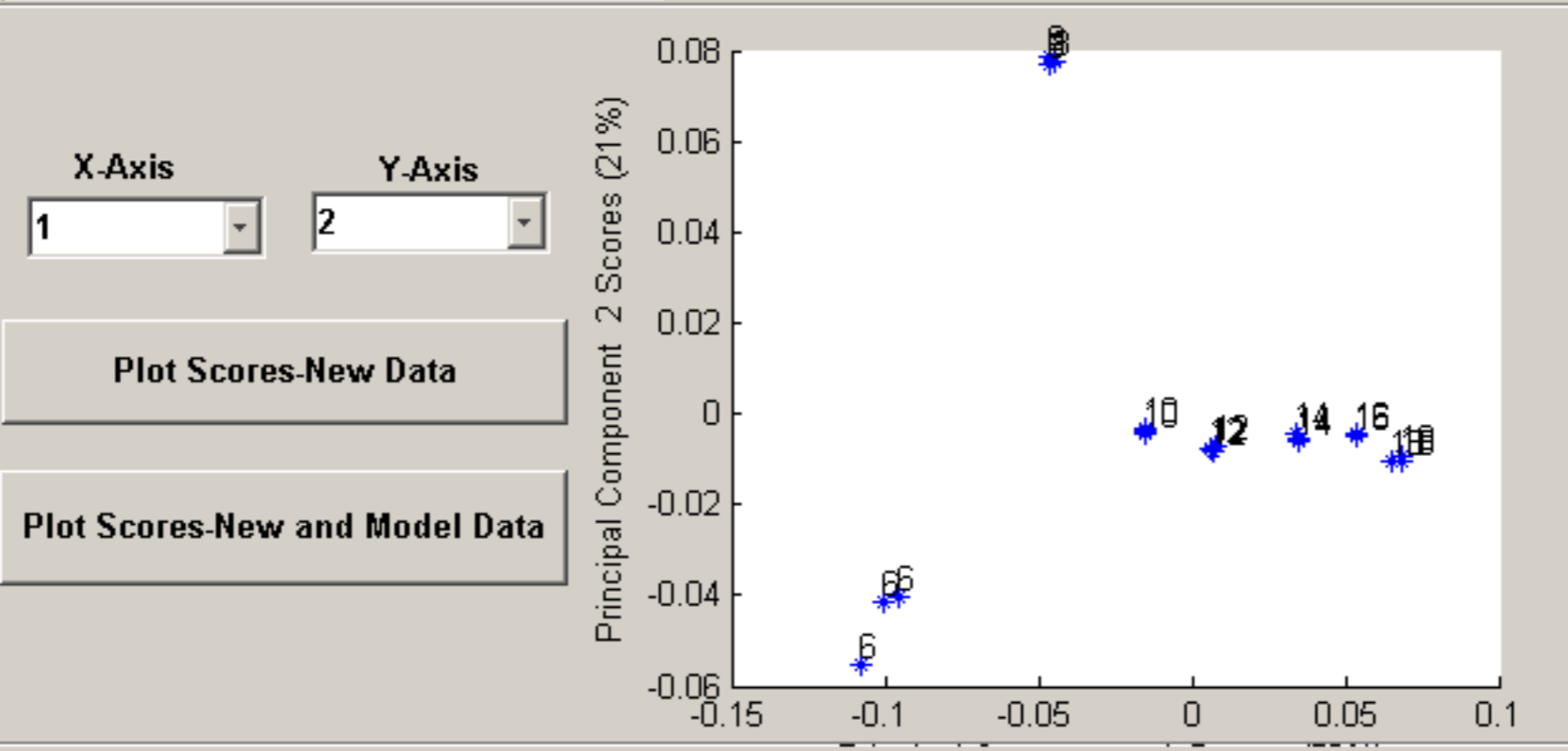
Data: **ndatass**
 Variables: **exactmass**
 Samples: **samplenames**

Model Data

Scores: **pcascores**
 Loads: **pca loads**
 % Variance: **pcavariance**
 Scaling Choice: **Mean Center**

New Data: **ntestdatass**

and press the 'Save Combined Scores' button.





Workspace



- Name ▲
- data
- exactmass
- filenames
- ndatass
- nommass
- ntestdatass
- samplenames
- testdata
- testfiles
- testsamples
- totalcounts

Command History

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Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise. Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix	Name of Variable Matrix	Name of Filename Matrix	Name of Totalcounts Matrix	Name of Samplenames Matrix
ndatass	exactmass	filenames	totalcounts	samplenames

That's it for this tutorial.

Press the green button on the left to go back to the previous step. Press the button the right to go back to the beginning of the tutorial.

