imagegui

File Data Pre Processing MVA Data Display Image Processing

## Data Selection Panel

**Name of Image Matrix** Select Data ...

**Name of Variable Matrix** Select Variables ...

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.

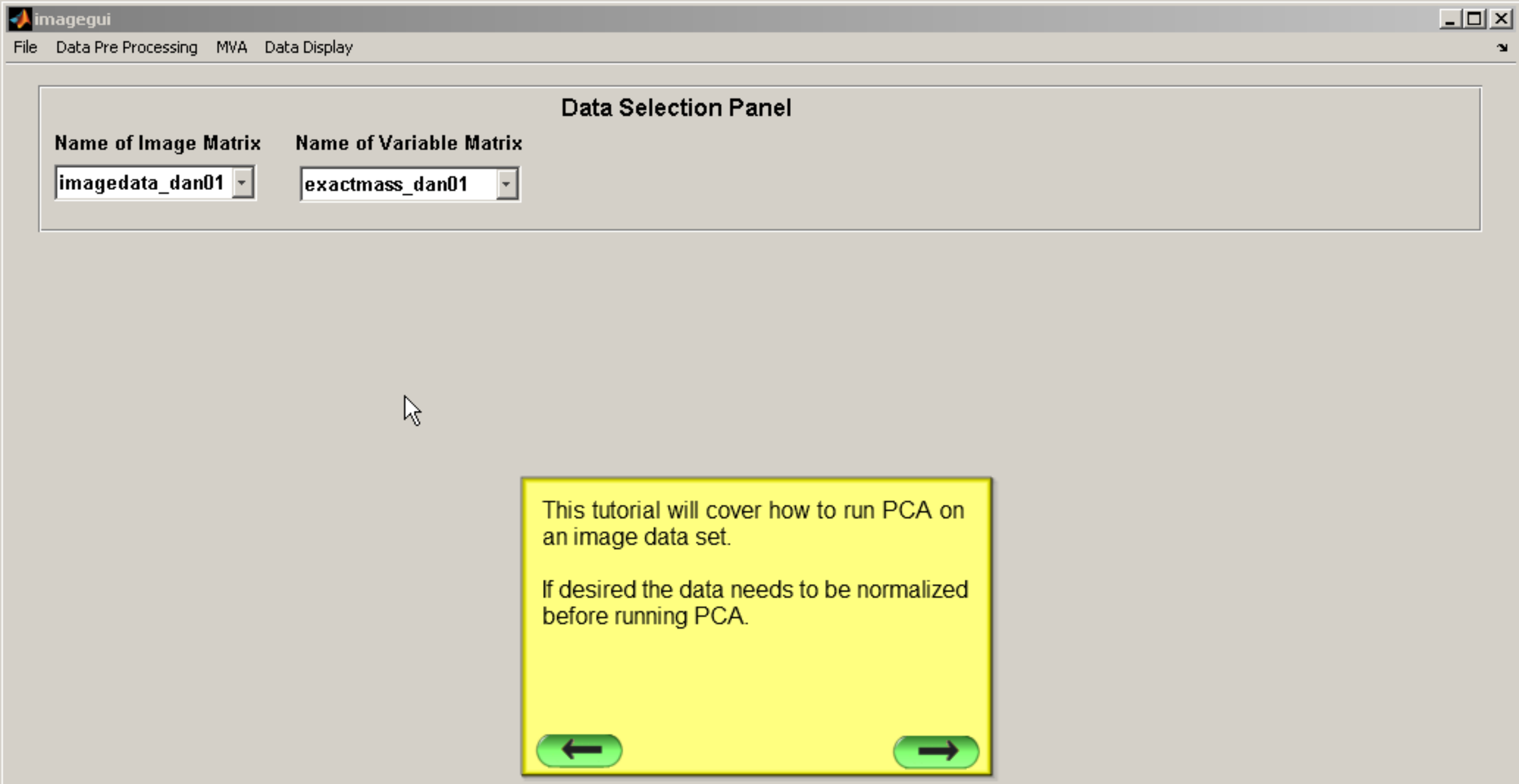
This is the 'Next' button. It takes you to the next frame or stop point.

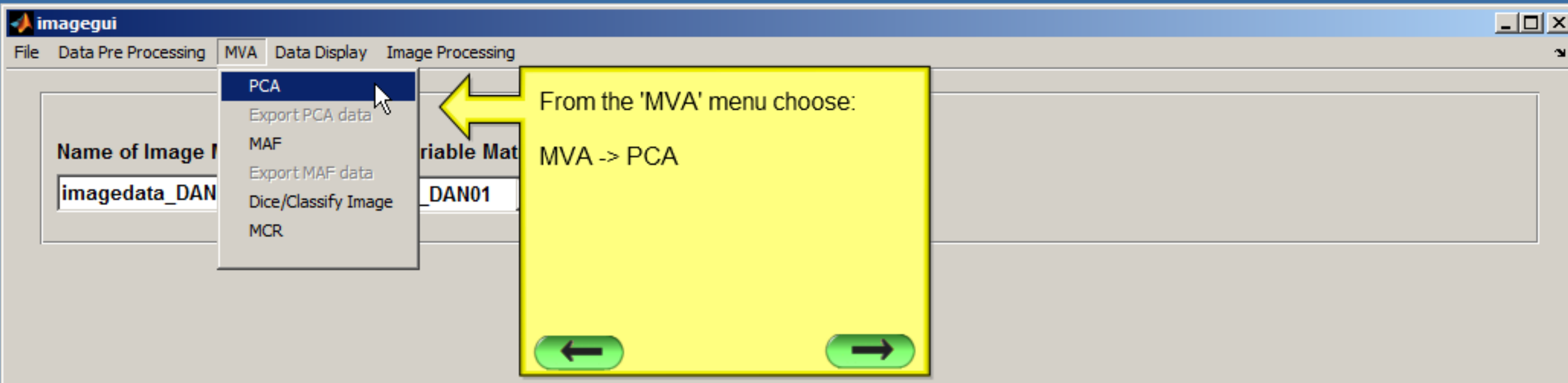
This is the 'Previous' button. It takes you to the previous frame or stop point.

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.


imagegui
File
Data Pre Processing
MVA
Data Display
Data Selection Panel
Name of Image Matrix
imagedata_dan01
Name of Variable Matrix
exactmass_dan01
This tutorial will cover how to run PCA on an image data set.
If desired the data needs to be normalized before running PCA.


imagegui
File
Data Pre Processing
MVA
Data Display
Image Processing
PCA
Export PCA data
MAF
Export MAF data
Dice/Classify Image
MCR
Name of Image I
riable Mat
imagedata_DAN
_DAN01
From the 'MVA' menu choose:
MVA -> PCA

imagegui

File Data Pre Processing MVA Data Display Image Processing

## Data Selection Panel

Name of Image Matrix: imagedata_DAN...

Name of Variable Matrix: exactmass_DAN01

Load Selected Data

Image: None

Variables None

This opens the Image PCA panel.

Data Preprocessing

Choose an option below

Run PCA

PCA Summary

PC# %Var %Vartotal

Name for scores matrix

Name for loadings matrix

Name for Variance matrix

# of PCs to keep in model

Save PCA Data

Close Panel

imagegui

File Data Pre Processing MVA Data Display Image Processing

## Data Selection Panel

Name of Image Matrix: imagedata_DAN...

Name of Variable Matrix: exactmass_DAN01

Load Selected Data

Image: None

Variables None

Press the 'Load Selected Data' button to load the data selected in the drop down menus above into the image PCA panel.

Data Preprocessing

Choose an option below

Run PCA

PCA Summary

PC# %Var %Vartotal

Name for scores matrix

Name for loadings matrix

Name for Variance matrix

# of PCs to keep in model

Save PCA Data

Close Panel

imagegui

File  Data Pre Processing  MVA  Data Display  Image Processing

## Data Selection Panel

**Name of Image Matrix**: imagedata_DAN...

**Name of Variable Matrix**: exactmass_DAN01

Load Selected Data

**Image:** imagedata_DAN01

**Variables** exactmass_DAN01

**Data Preprocessing**

Choose an option below

- Choose an option below
- None
- Autoscale
- Mean Center
- Squareroot
- Squareroot & mean center
- Poisson Scaling
- PoissonScaling & Mean Center
- Mass scale
- Mass scale & Mean Center
- Mass^2 scale
- Mass^2 scale & Mean Center

**Name for scores matrix**

**Name for loadings matrix**

**Name for Variance matrix**

**# of PCs to keep in model**

Save PCA Data

Choose a preprocessing option from the 'Data Preprocessing' drop down menu.

These option are included to allow the user to explore different data preprocessing methods. Their inclusion herein does not denote a recommendation or suggestion on how to process SIMS image data.

The options include:
None - do not carry out any preprocessing

Autoscale - autoscale the data. This mean centers the data and then divides by the variance of each variable. Autoscaling is not recommended for image data.

Mean Center - Mean centers the data by subtracting the variable means from each variable.

Squareroot mean center - takes the squareroot of the data and then mean centers the data.

Poisson scaling - scales the data according to the method developed by Keenan and Kotula (Appl. Surf. Sci. 231-232 (2004) 240-244)

Mass scale - scales each peak area by multiplying by the mass of the peak.

Mass^2 scale - scales each peak area by the mass of the peak squared .

Many of the above methods also include an option to mean center after doing the respective scaling or transformation.

imagegui

File Data Pre Processing MVA Data Display Image Processing

## Data Selection Panel

**Name of Image Matrix** imagedata_DAN...

**Name of Variable Matrix** exactmass_DAN01

Load Selected Data

**Image:** imagedata_DAN01

**Variables** exactmass_DAN01

**Data Preprocessing**

Choose an option below

- Choose an option below
- None
- Autoscale
- Mean Center
- Squareroot
- Squareroot & mean center
- Poisson Scaling
- PoissonScaling & Mean Center
- Mass scale
- Mass scale & Mean Center
- Mass^2 scale
- Mass^2 scale & Mean Center

Here we will choose 'Poisson Scaling & Mean Center'

**Name for scores matrix**

**Name for loadings matrix**

**Name for Variance matrix**

**# of PCs to keep in model**

Save PCA Data

Close Panel

imagegui

File Data Pre Processing MVA Data Display Image Processing

## Data Selection Panel

Name of Image Matrix: imagedata_DAN...

Name of Variable Matrix: exactmass_DAN01

Load Selected Data

Image: imagedata_DAN01

Variables exactmass_DAN01

Data Preprocessing

Choose an option below

Run PCA

Press the 'Run PCA' button to carry out PCA on the selected data.

PCA Summary

PC# %Var %Vartotal

Name for scores matrix

Name for loadings matrix

Name for Variance matrix

# of PCs to keep in model

Save PCA Data

Close Panel

imagegui

File Data Pre Processing MVA Data Display Image Processing

## Data Selection Panel

Name of Image Matrix: imagedata_DAN...

Name of Variable Matrix: exactmass_DAN01

Load Selected Data

Image: imagedata_DAN01

Variables exactmass_DAN01

Data Preprocessing

PoissonScaling & Mean Center

Run PCA

PCA Summary

| PC# | %Var | %Vartotal |
|---|---|---|
| 1 | 35.8 | 35.8 |
| 2 | 6.1 | 41.9 |
| 3 | 4.6 | 46.5 |
| 4 | 3.8 | 50.3 |
| 5 | 3.7 | 54 |
| 6 | 3.6 | 57.6 |
| 7 | 3.5 | 61.1 |
| 8 | 3.5 | 64.6 |
| 9 | 3.4 | 68 |
| 10 | 3.4 | 71.4 |

Name for scores matrix

Name for loadings matrix

Name for Variance matrix

# of PCs to keep in model

Save PCA Data

PC #: Choose one

Plot Scores and Loads

Split Pos/Neg S&L

Opens a separate figure window

Browse all PCA plots

Opens a separate figure window

number PCs for Grid

A summary of the variance captured per PC is shown in the table. New boxes appear that enable looking at the scores and loadings.

Close Panel

imagegui

File Data Pre Processing MVA Data Display Image Processing

## Data Selection Panel

Name of Image Matrix: imagedata_DAN...

Name of Variable Matrix: exactmass_DAN01

Load Selected Data

Image: imagedata_DAN01

Variables exactmass_DAN01

Data Preprocessing

Poisson Scaling & Mean Center

Run PCA

PCA Summary

| PC# | %Var | %Vartotal |
|---|---|---|
| 1 | 35.8 | 35.8 |
| 2 | 6.1 | 41.9 |
| 3 | 4.6 | 46.5 |
| 4 | 3.8 | 50.3 |
| 5 | 3.7 | 54 |
| 6 | 3.6 | 57.6 |
| 7 | 3.5 | 61.1 |
| 8 | 3.5 | 64.6 |
| 9 | 3.4 | 68 |
| 10 | 3.4 | 71.4 |

Name for scores matrix

Name for loadings matrix

Name for Variance matrix

# of PCs to keep in model

Save PCA Data

PC #

Choose one

Choose one, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19

Opens a separate figure window

To see a score and loading plot choose the desired PC number from the drop down menu.

Close Panel

imagegui

File Data Pre Processing MVA Data Display Image Processing

## Data Selection Panel

Name of Image Matrix: imagedata_DAN...

Name of Variable Matrix: exactmass_DAN01

Load Selected Data

Image: imagedata_DAN01

Variables exactmass_DAN01

Data Preprocessing

Poisson Scaling & Mean Center

Run PCA

PCA Summary

| PC# | %Var | %Vartotal |
|---|---|---|
| 1 | 35.8 | 35.8 |
| 2 | 6.1 | 41.9 |
| 3 | 4.6 | 46.5 |
| 4 | 3.8 | 50.3 |
| 5 | 3.7 | 54 |
| 6 | 3.6 | 57.6 |
| 7 | 3.5 | 61.1 |
| 8 | 3.5 | 64.6 |
| 9 | 3.4 | 68 |
| 10 | 3.4 | 71.4 |

Name for scores matrix

Name for loadings matrix

Name for Variance matrix

# of PCs to keep in model

Save PCA Data

PC #: 1

Plot Scores and Loads

Split Pos/Neg S&L

Opens a separate figure window

Browse all PCA plots

Opens a separate figure window

number PCs for Grid

Plot Multiple PCs in Grid

Opens a separate figure window

And press the 'Plot Scores and Loads' button.

Close Panel

imagegui

File Data Pre Processing MVA Data Display Image Processing

## Data Selection Panel

Name of Image Matrix: imagedata_DAN...

Name of Variable Matrix: exactmass_DAN01

Load Selected Data

Image: imagedata_DAN01

Variables exactmass_DAN01

Data Preprocessing

Poisson Scaling & Mean Center

Run PCA

| PC# | PCA %Var | Su % |
|---|---|---|
| 1 | 35.8 | |
| 2 | 6.1 | |
| 3 | 4.6 | |
| 4 | 3.8 | |
| 5 | 3.7 | |
| 6 | 3.6 | 57.6 |
| 7 | 3.5 | 61.1 |
| 8 | 3.5 | 64.6 |
| 9 | 3.4 | 68 |
| 10 | 3.4 | 71.4 |

Name for scores matrix

Name for loadings matrix

Name for Variance matrix

# of PCs to keep in model

Save PCA Data

PC #: 1

Plot Scores and Loads

Split Pos/Neg S&L

Opens a separate figure window

Browse all PCA plots

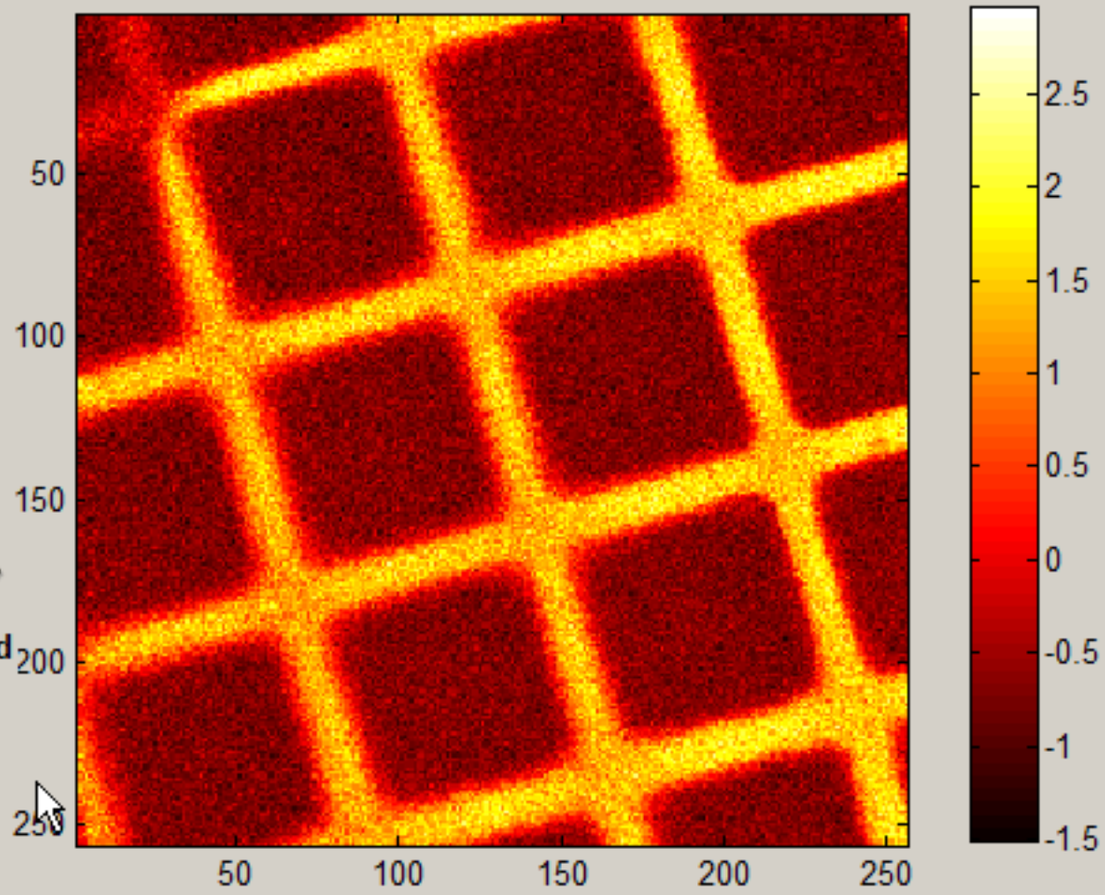
ate

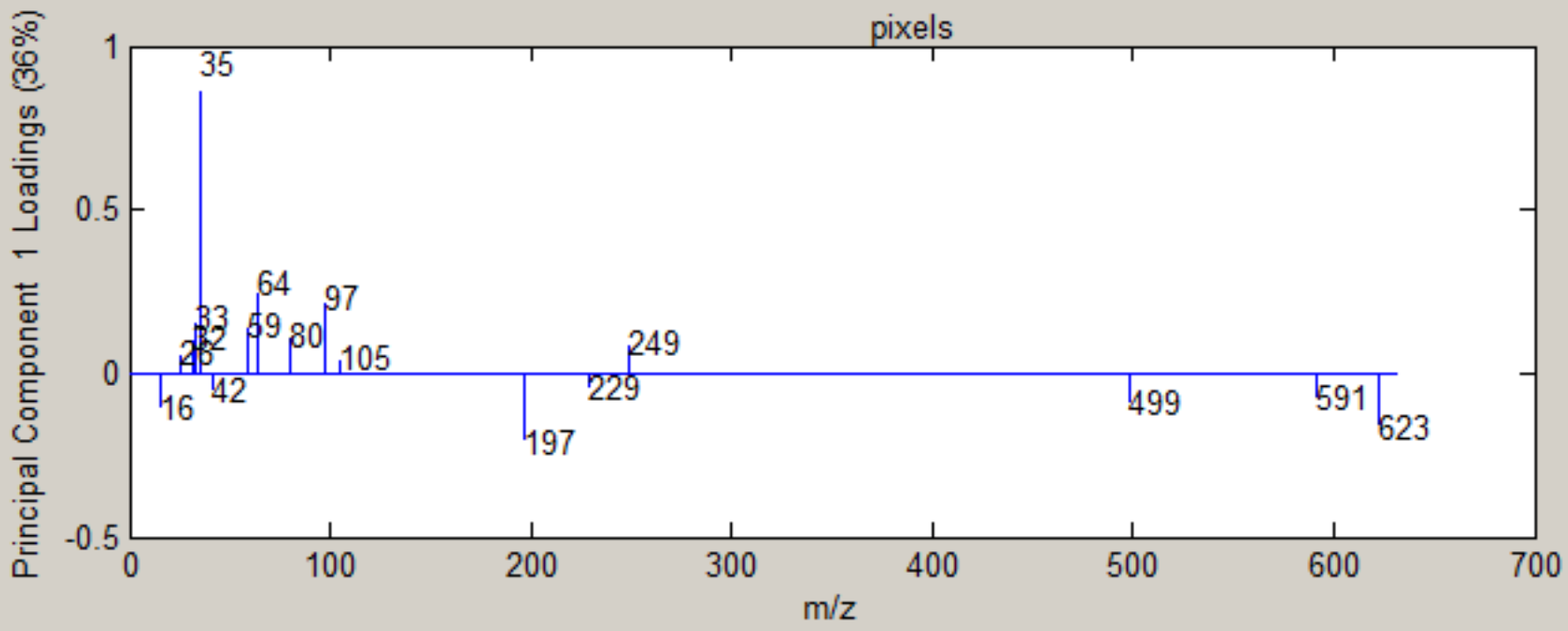
s for Grid

in Grid

ate

The scores and loadings for the selected variable are shown in the plots on the right.




Close Panel

imagegui

File Data Pre Processing MVA Data Display Image Processing

## Data Selection Panel

Name of Image Matrix: imagedata_DAN...

Name of Variable Matrix: exactmass_DAN01

Load Selected Data

Image: imagedata_DAN01

Variables exactmass_DAN01

Data Preprocessing

Poisson Scaling & Mean Center

Run PCA

PCA Summary

| PC# | %Var | %Vartotal |
|---|---|---|
| 1 | 35.8 | 35.8 |
| 2 | 6.1 | 41.9 |
| 3 | 4.6 | 46.5 |
| 4 | 3.8 | 50.3 |
| 5 | 3.7 | 54 |
| 6 | 3.6 | 57.6 |
| 7 | 3.5 | 61.1 |
| 8 | 3.5 | 64.6 |
| 9 | 3.4 | 68 |
| 10 | 3.4 | 71.4 |

Name for scores matrix

Name for loadings matrix

Name for Variance matrix

# of PCs to keep in model

Save PCA Data

PC #: 1

Plot Scores and Loads

Split Pos/Neg S&L

Opens a separate figure window

Browse all PCA plots

Opens a separate figure window

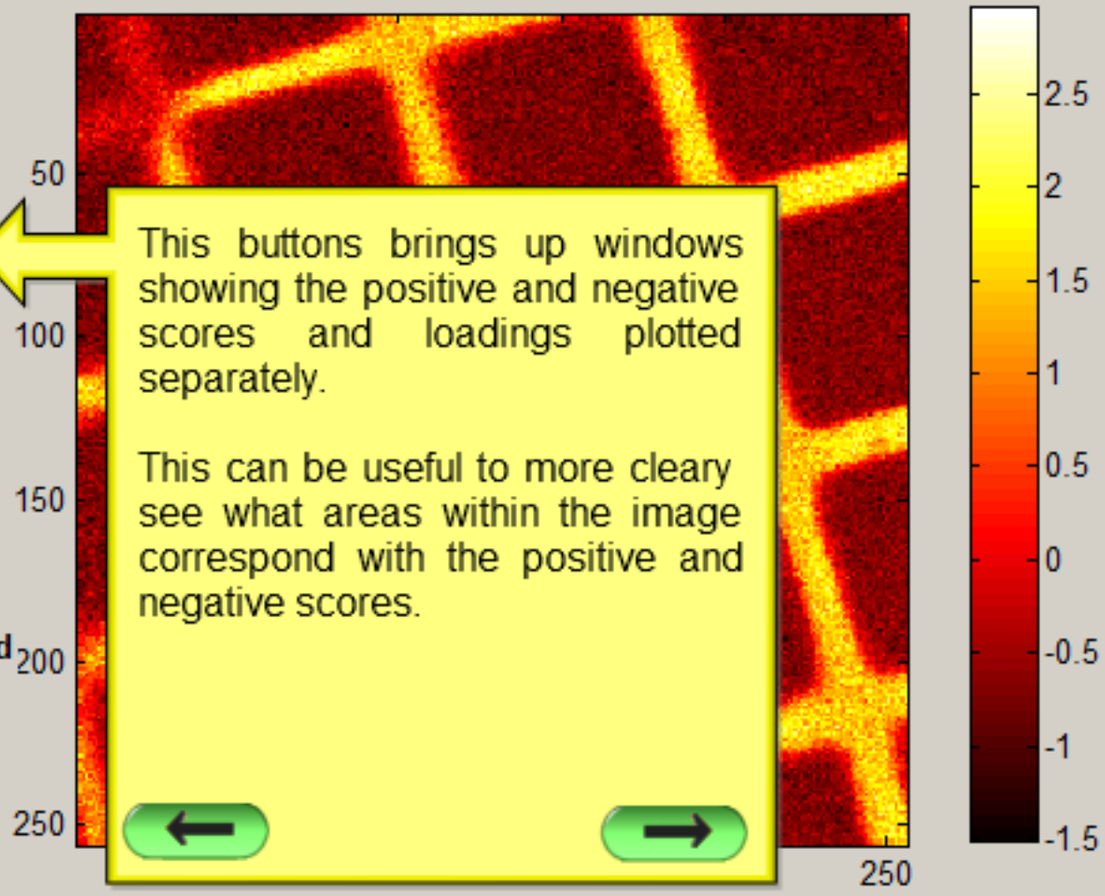
number PCs for Grid

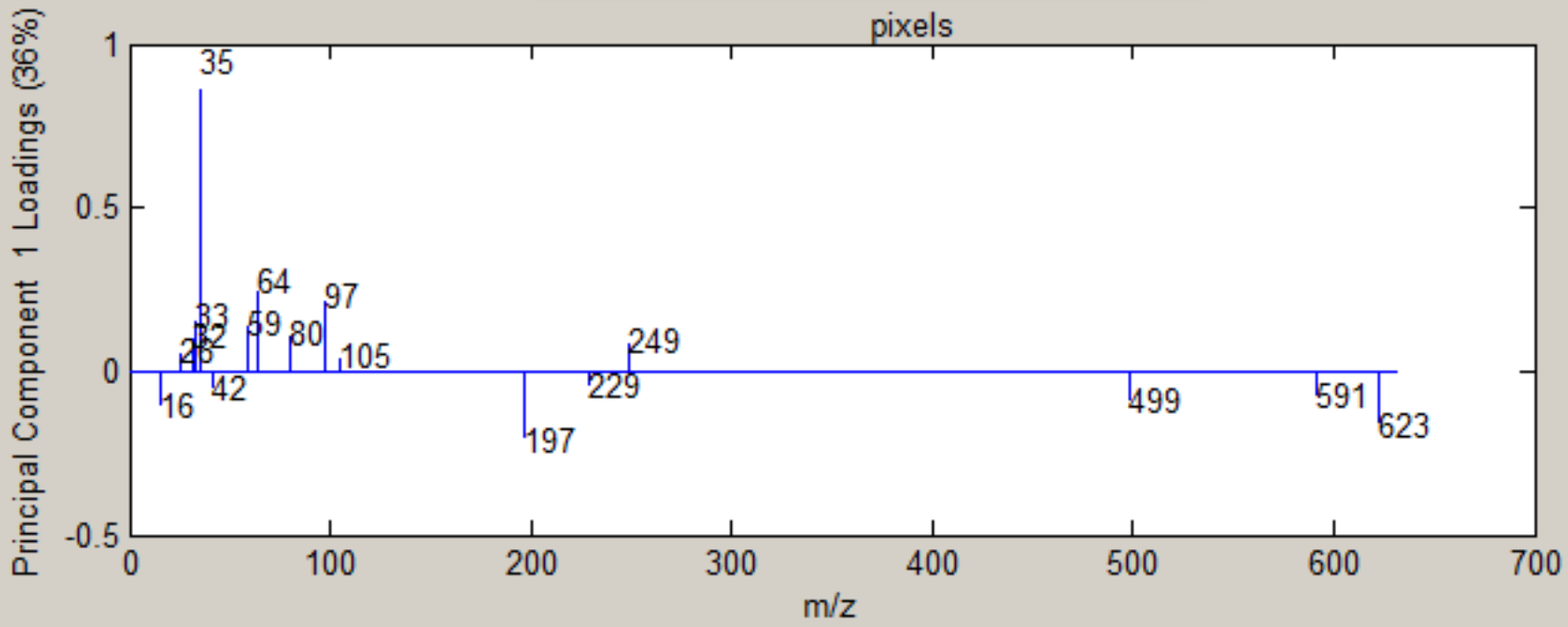
Plot Multiple PCs in Grid

Opens a separate figure window

This buttons brings up windows showing the positive and negative scores and loadings plotted separately.

This can be useful to more cleary see what areas within the image correspond with the positive and negative scores.

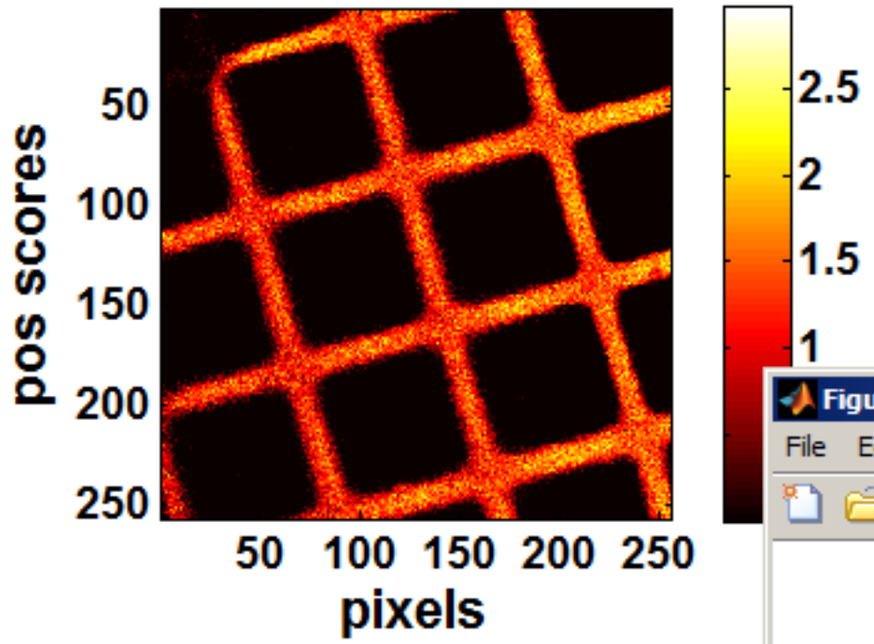



Close Panel

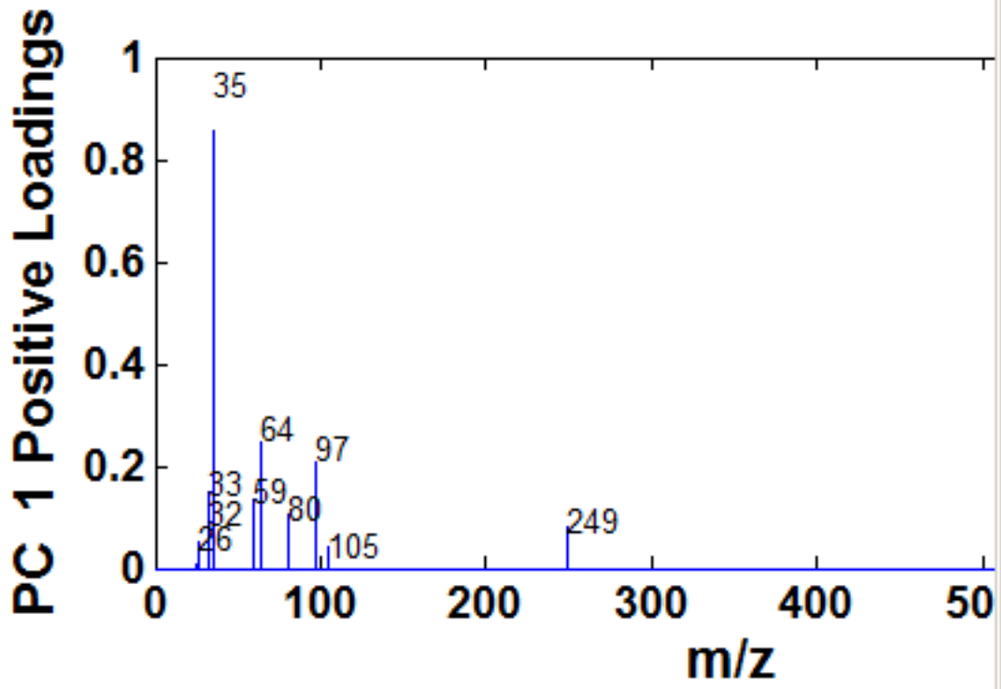
Figure 1

File Edit View Insert Tools Desktop Window Help










Name for loadings matrix

Name for Variance matrix

# of PCs to keep in model

Save PCA Data

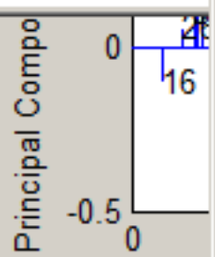
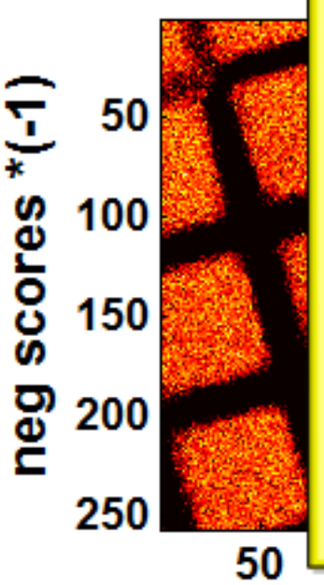



Figure 2

File Edit View Insert Tools Desktop



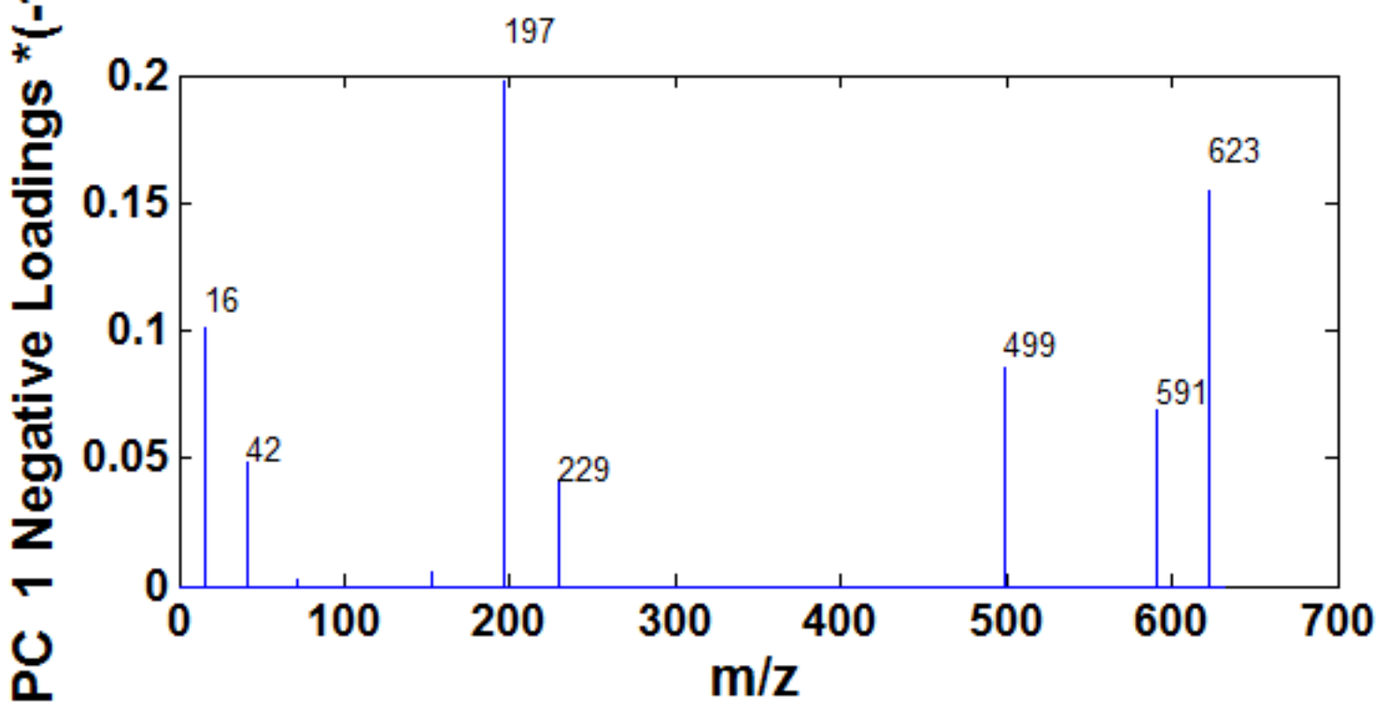


Here is an example of what the positive and negative scores and loadings look like.

In these plots the negative scores and loadings have been multiplied by -1 in order to display them on a typical color scale starting at zero.

This transformation is only done for the data display and does not affect the original scores or loadings.

Such transformations are okay as long as you always multiply the scores and loadings by the same value.



imagegui

File Data Pre Processing MVA Data Display Image Processing

## Data Selection Panel

**Name of Image Matrix** imagedata_DAN...

**Name of Variable Matrix** exactmass_DAN01

Load Selected Data

**Image:** imagedata_DAN01

**Variables** exactmass_DAN01

**Data Preprocessing**

Poisson Scaling & Mean Center

Run PCA

**PCA Summary**

| PC# | %Var | %Vartotal |
|---|---|---|
| 1 | 35.8 | 35.8 |
| 2 | 6.1 | 41.9 |
| 3 | 4.6 | 46.5 |
| 4 | 3.8 | 50.3 |
| 5 | 3.7 | 54 |
| 6 | 3.6 | 57.6 |
| 7 | 3.5 | 61.1 |
| 8 | 3.5 | 64.6 |
| 9 | 3.4 | 68 |
| 10 | 3.4 | 71.4 |

**Name for scores matrix**

**Name for loadings matrix**

**Name for Variance matrix**

**# of PCs to keep in model**

Save PCA Data

**PC #** 1

Plot Scores and Loads

Split Pos/Neg S&L

Opens a separate figure window

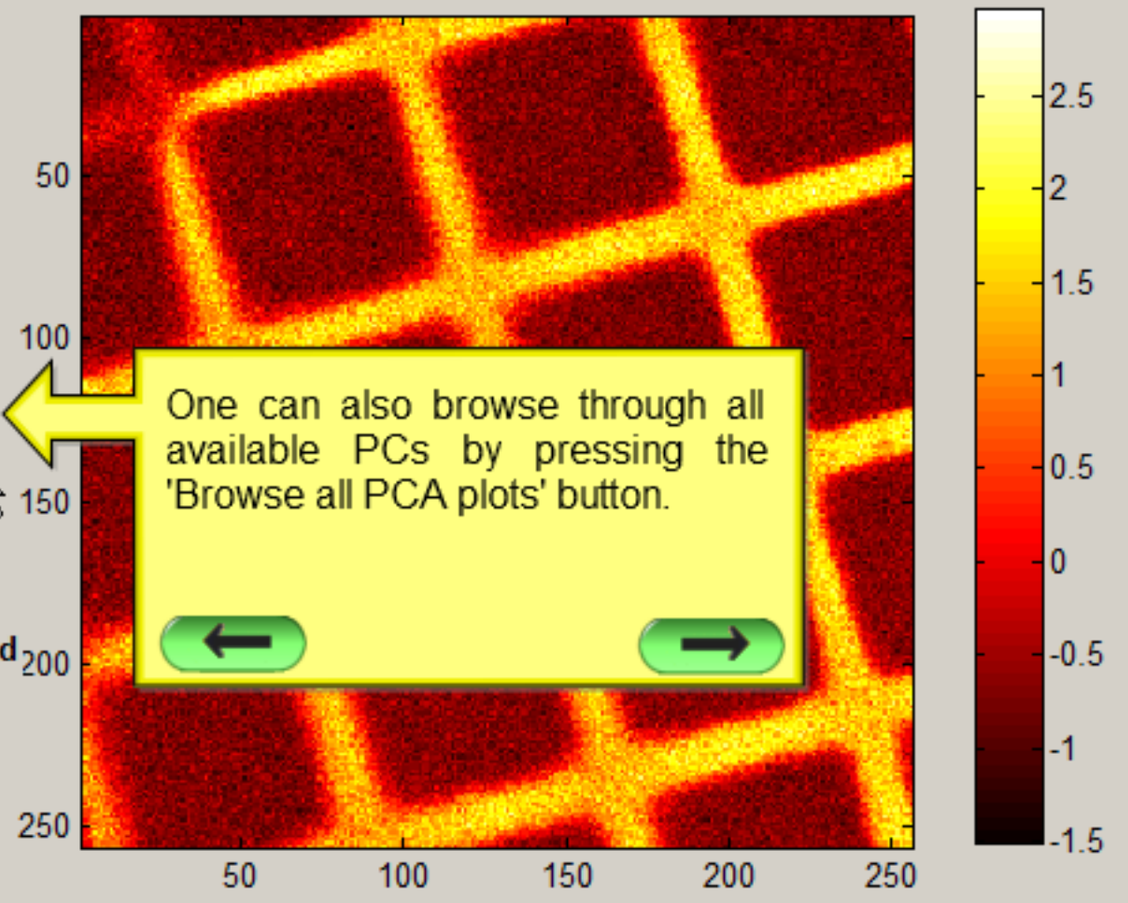
Browse all PCA plots

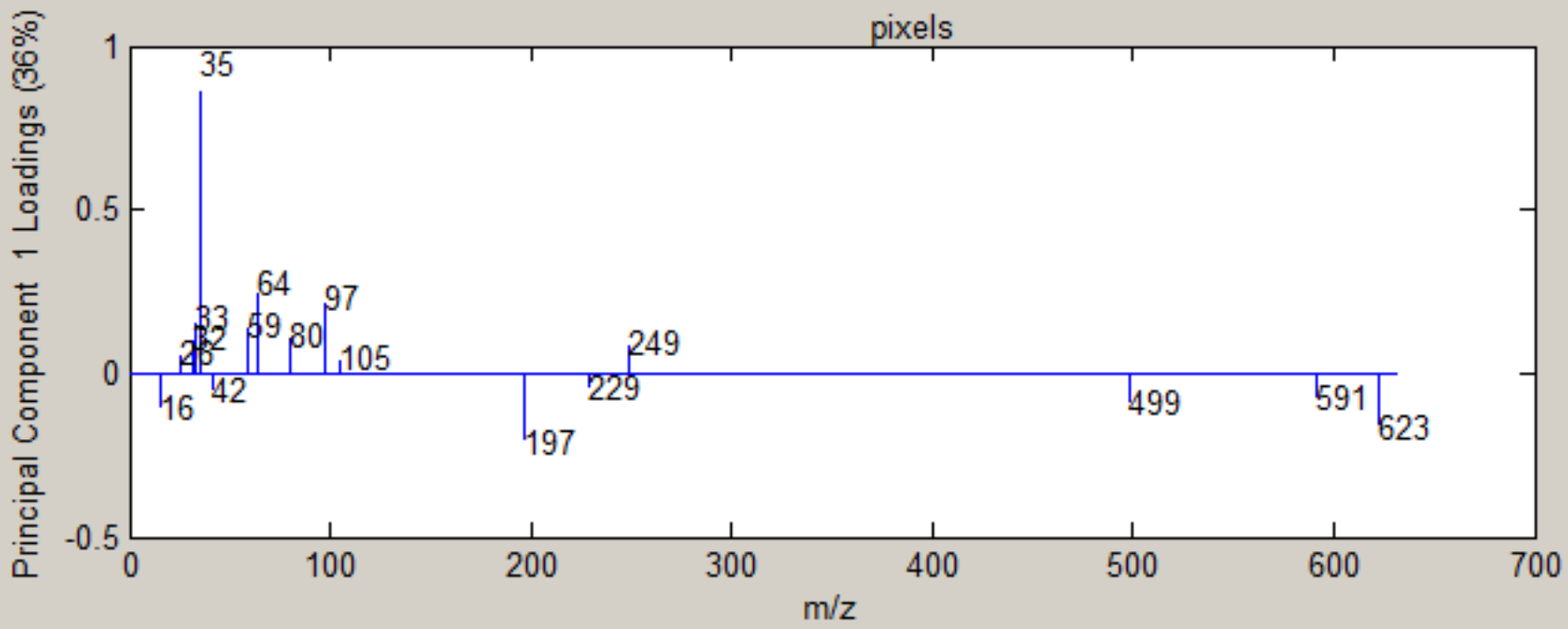
Opens a separate figure window

number PCs for Grid

Plot Multiple PCs in Grid

Opens a separate figure window




Close Panel

imagegui

File Data Pre Processing MVA Data Display Image Processing

## Data Selection Panel

Name of Image Matrix

imagedata_DAN...

Load Selected I

Image: imaged

This brings up an additional window. By left clicking anywhere in the window it will automatically cycle through all available PC scores and loading plots.

Run PCA

PCA Summ

| PC# | %Var | %Var |
|---|---|---|
| 1 | 35.8 | |
| 2 | 6.1 | |
| 3 | 4.6 | |
| 4 | 3.8 | |
| 5 | 3.7 | |
| 6 | 3.6 | |
| 7 | 3.5 | |
| 8 | 3.5 | |
| 9 | 3.4 | |
| 10 | 3.4 | |

Name for scores

Name for loadings

Name for Variance

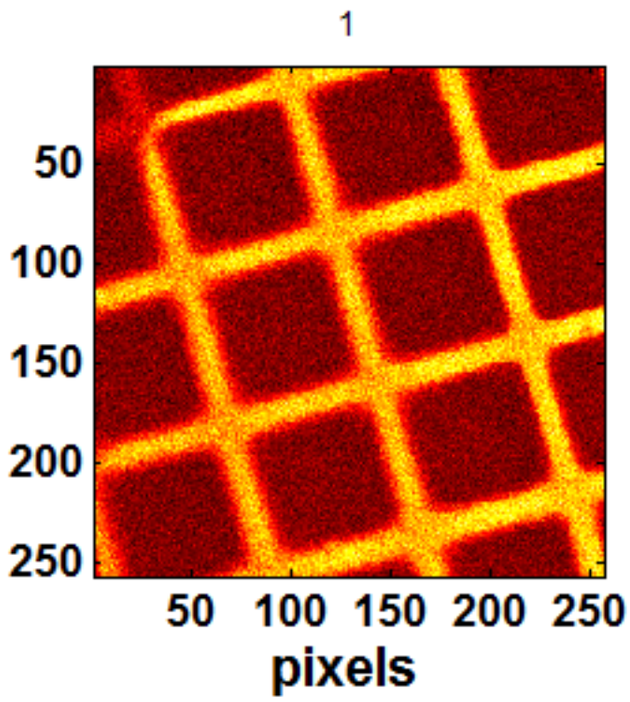
# of PCs to keep in model

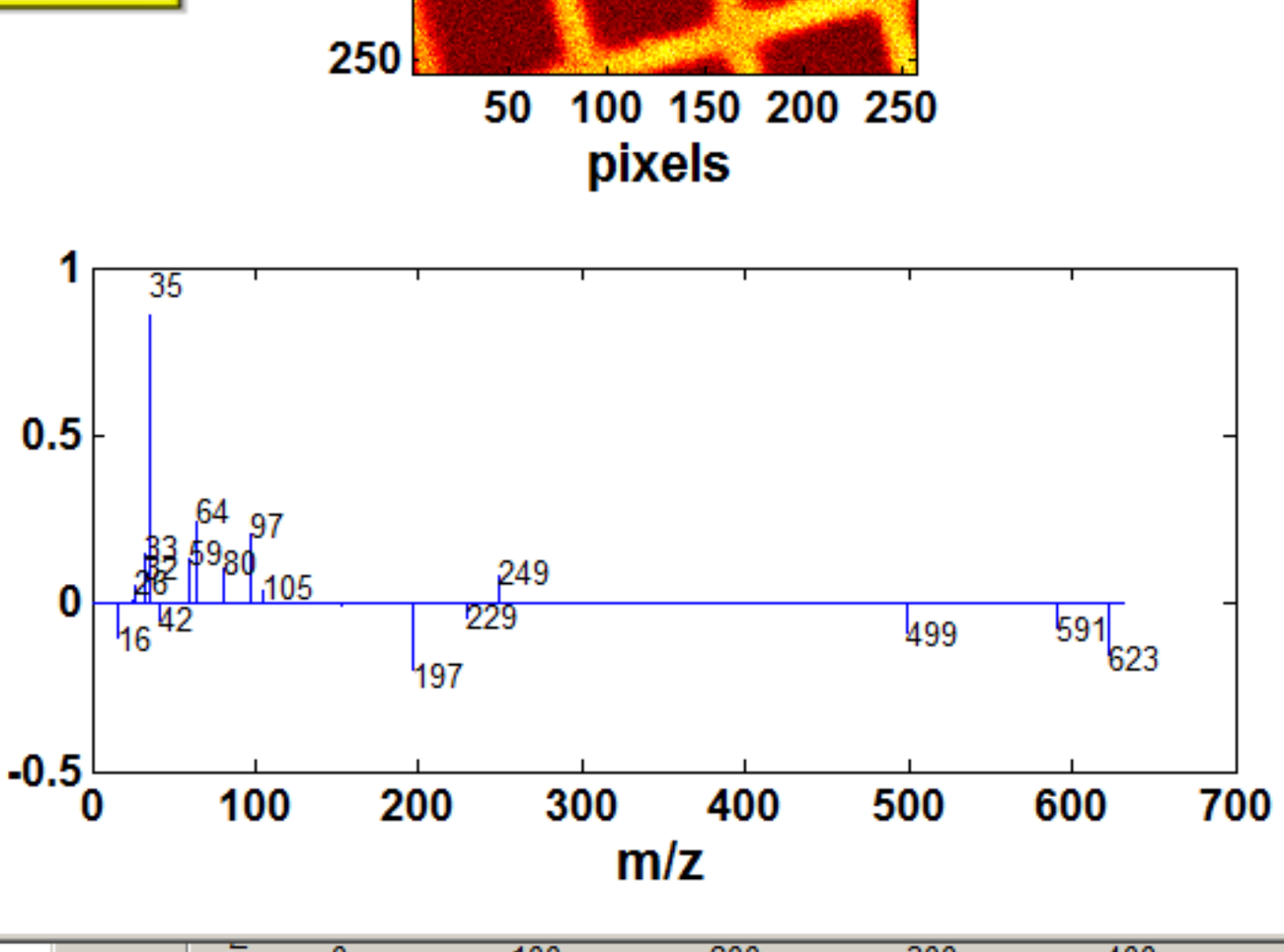
Save PCA Data

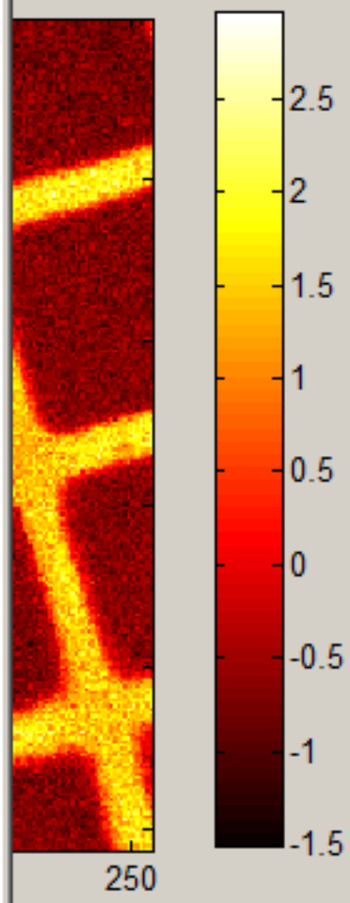
Close Panel

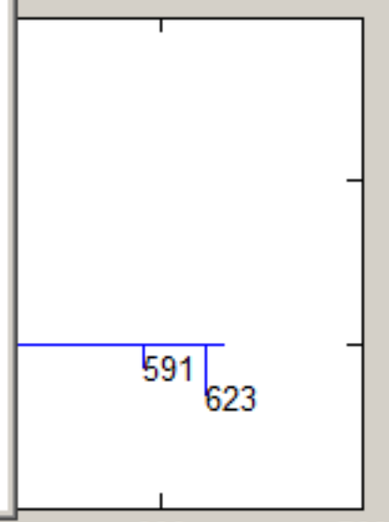
Figure 1

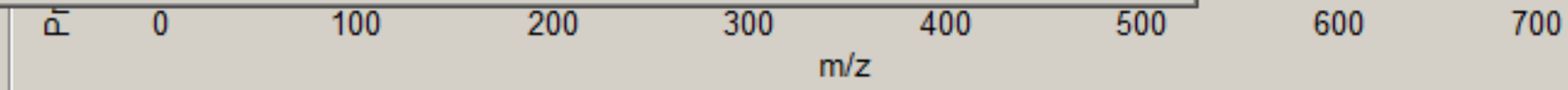
File Edit View Insert Tools Desktop Window Help



imagegui

File Data Pre Processing MVA Data Display Image Processing

## Data Selection Panel

Name of Image Matrix

imagedata_DAN...

Load Selected I

Image: imaged

Each mouse click updates the window with the next PC

Run PCA

| PC# | %Var | PCA Summ %Var |
|---|---|---|
| 1 | 35.8 | |
| 2 | 6.1 | |
| 3 | 4.6 | |
| 4 | 3.8 | |
| 5 | 3.7 | |
| 6 | 3.6 | |
| 7 | 3.5 | |
| 8 | 3.5 | |
| 9 | 3.4 | |
| 10 | 3.4 | |

Name for scores

Name for loadings

Name for Variance

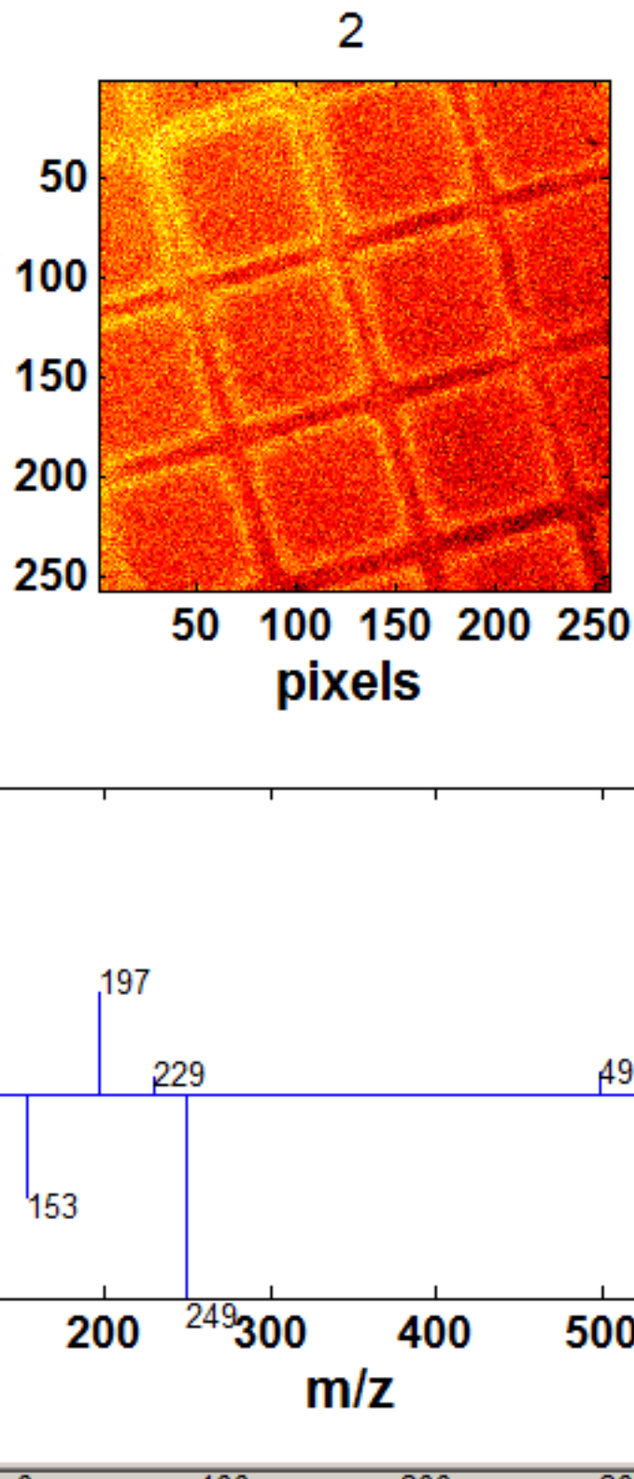
# of PCs to keep in model

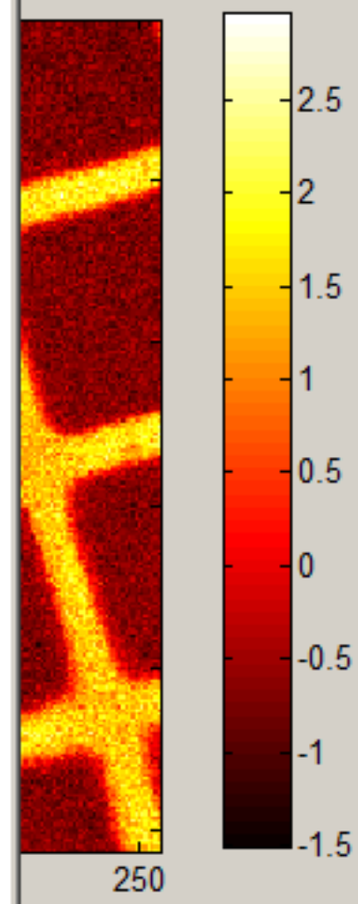
Save PCA Data

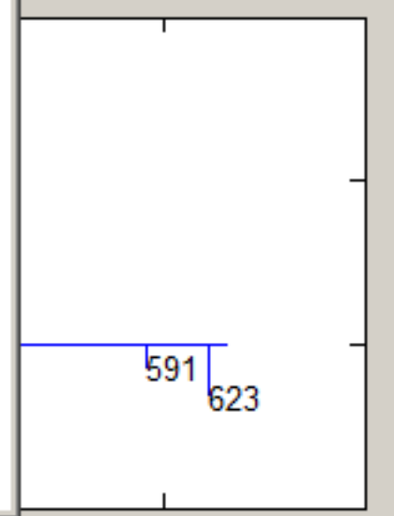
Close Panel

Figure 1

File Edit View Insert Tools Desktop Window Help



imagegui

File Data Pre Processing MVA Data Display Image Processing

## Data Selection Panel

Name of Image Matrix

imagedata_DAN...

Load Selected I

Image: imaged

Variables exactm

Data Preproces

PoissonScaling & Mean Cent

Run PCA

| PC# | %Var | PCA Summ %Var |
|---|---|---|
| 1 | 35.8 | |
| 2 | 6.1 | |
| 3 | 4.6 | |
| 4 | 3.8 | |
| 5 | 3.7 | |
| 6 | 3.6 | |
| 7 | 3.5 | |
| 8 | 3.5 | |
| 9 | 3.4 | |
| 10 | 3.4 | |

Name for scores

Name for loadings

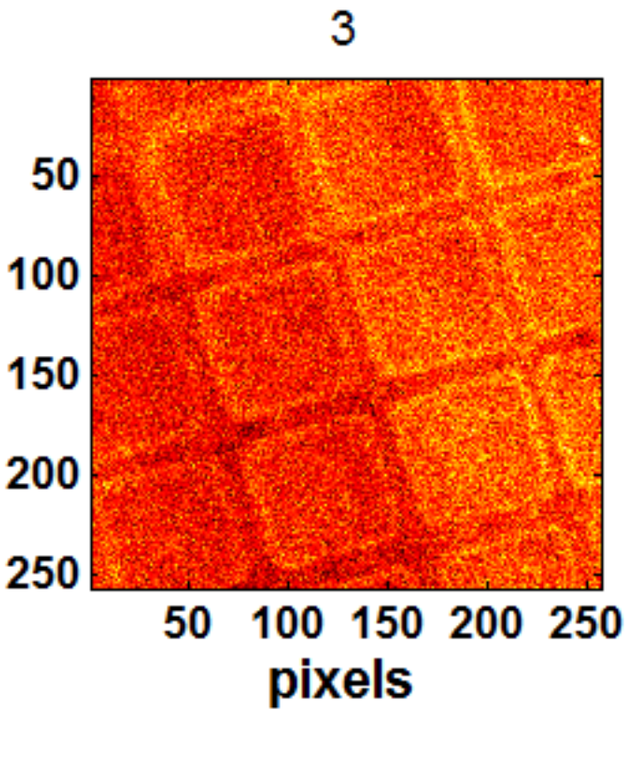
Name for Variance

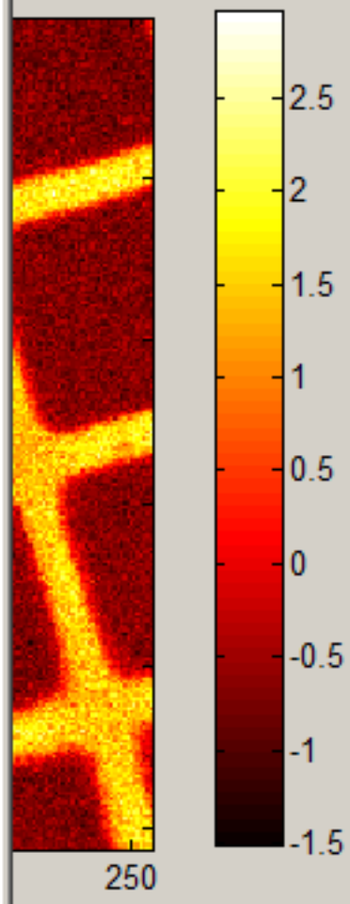
# of PCs to keep in model

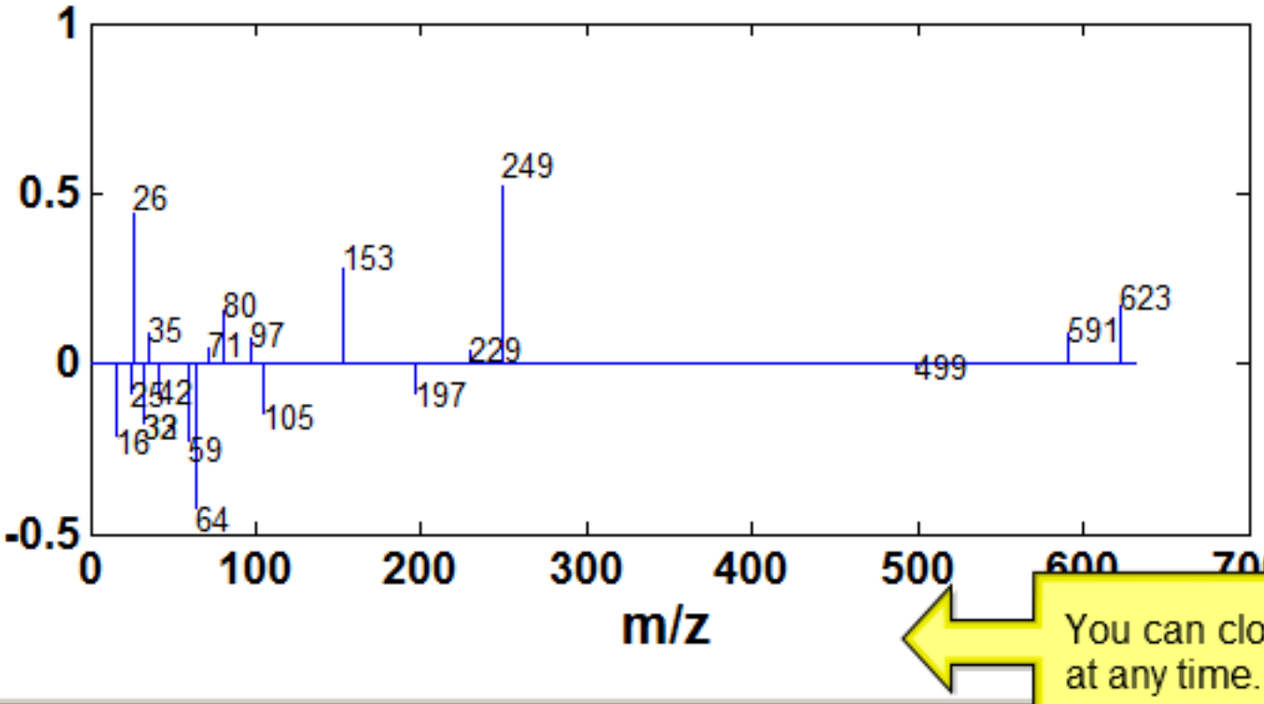
Save PCA Data

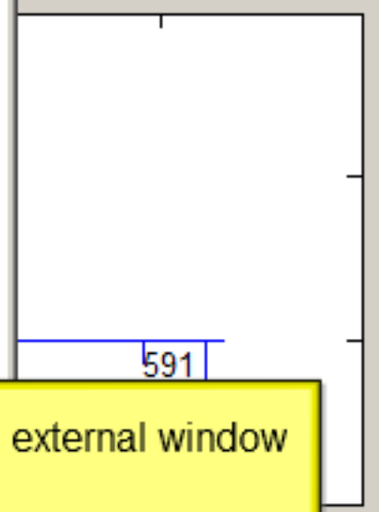
Figure 1

File Edit View Insert Tools Desktop Window Help




You can close this external window at any time.

Close Panel

imagegui

File Data Pre Processing MVA Data Display Image Processing

## Data Selection Panel

**Name of Image Matrix** imagedata_DAN...

**Name of Variable Matrix** exactmass_DAN01

Load Selected Data

**Image:** imagedata_DAN01

**Variables** exactmass_DAN01

**Data Preprocessing**

Poisson Scaling & Mean Center

Run PCA

**PCA Summary**

| PC# | %Var | %Vartotal |
|---|---|---|
| 1 | 35.8 | 35.8 |
| 2 | 6.1 | 41.9 |
| 3 | 4.6 | 46.5 |
| 4 | 3.8 | 50.3 |
| 5 | 3.7 | 54 |
| 6 | 3.6 | 57.6 |
| 7 | 3.5 | 61.1 |
| 8 | 3.5 | 64.6 |
| 9 | 3.4 | 68 |
| 10 | 3.4 | 71.4 |

**Name for scores matrix**

**Name for loadings matrix**

**Name for Variance matrix**

**# of PCs to keep in model**

Save PCA Data

**PC #** 1

Plot Scores and Loads

Split Pos/Neg S&L

Opens a separate figure window

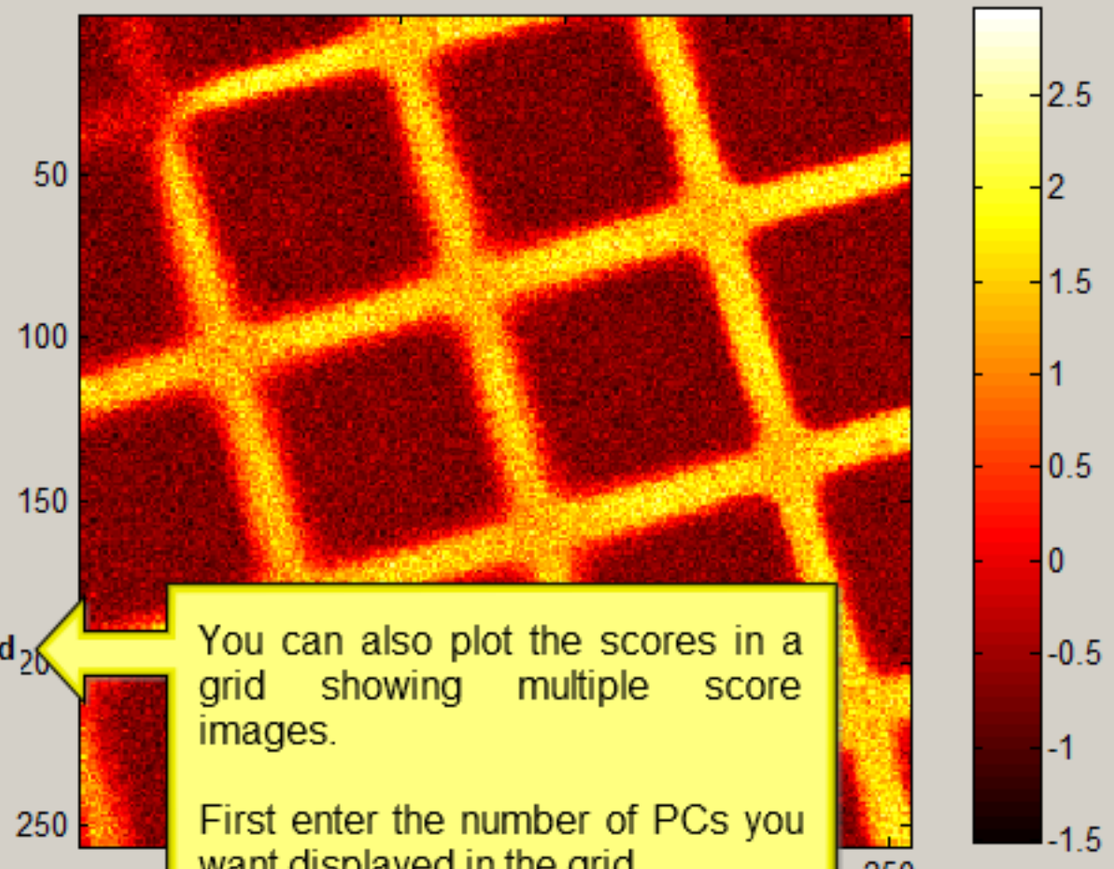
Browse all PCA plots

Opens a separate figure window

4 number PCs for Grid

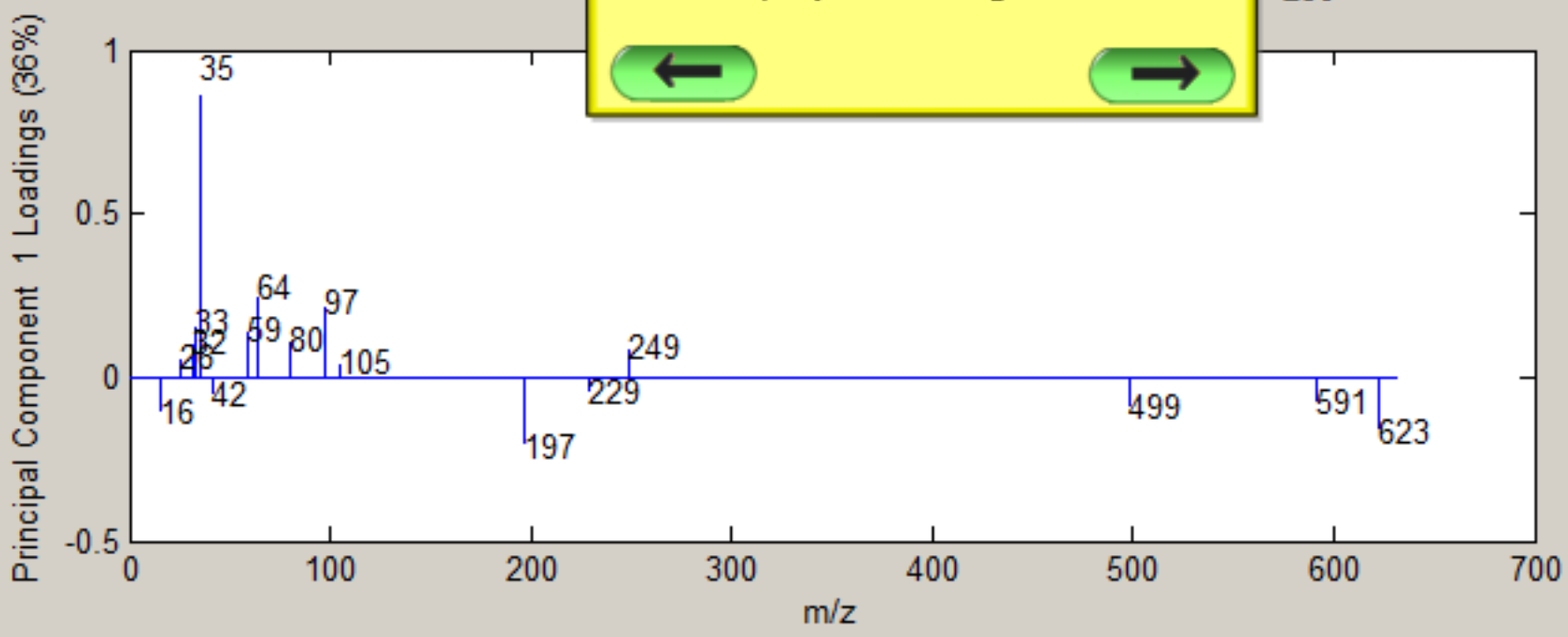
Plot Multiple PCs in Grid

Opens a separate figure window




You can also plot the scores in a grid showing multiple score images.

First enter the number of PCs you want displayed in the grid.




Close Panel

imagegui

File  Data Pre Processing  MVA  Data Display  Image Processing

## Data Selection Panel

Name of Image Matrix: imagedata_DAN...

Name of Variable Matrix: exactmass_DAN01

Load Selected Data

Image: imagedata_DAN01

Variables exactmass_DAN01

Data Preprocessing

Poisson Scaling & Mean Center

Run PCA

PCA Summary

| PC# | %Var | %Vartotal |
|---|---|---|
| 1 | 35.8 | 35.8 |
| 2 | 6.1 | 41.9 |
| 3 | 4.6 | 46.5 |
| 4 | 3.8 | 50.3 |
| 5 | 3.7 | 54 |
| 6 | 3.6 | 57.6 |
| 7 | 3.5 | 61.1 |
| 8 | 3.5 | 64.6 |
| 9 | 3.4 | 68 |
| 10 | 3.4 | 71.4 |

Name for scores matrix

Name for loadings matrix

Name for Variance matrix

# of PCs to keep in model

Save PCA Data

PC #: 1

Plot Scores and Loads

Split Pos/Neg S&L

Opens a separate figure window

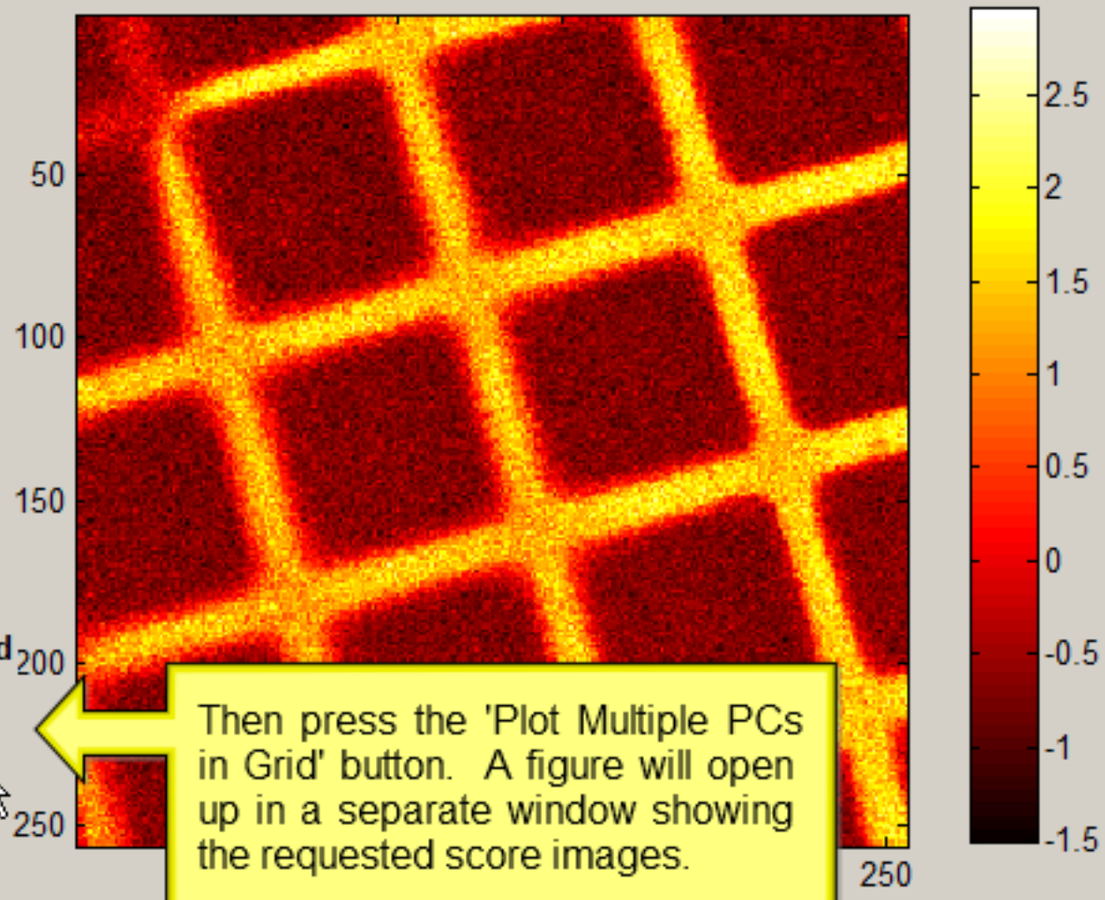
Browse all PCA plots

Opens a separate figure window

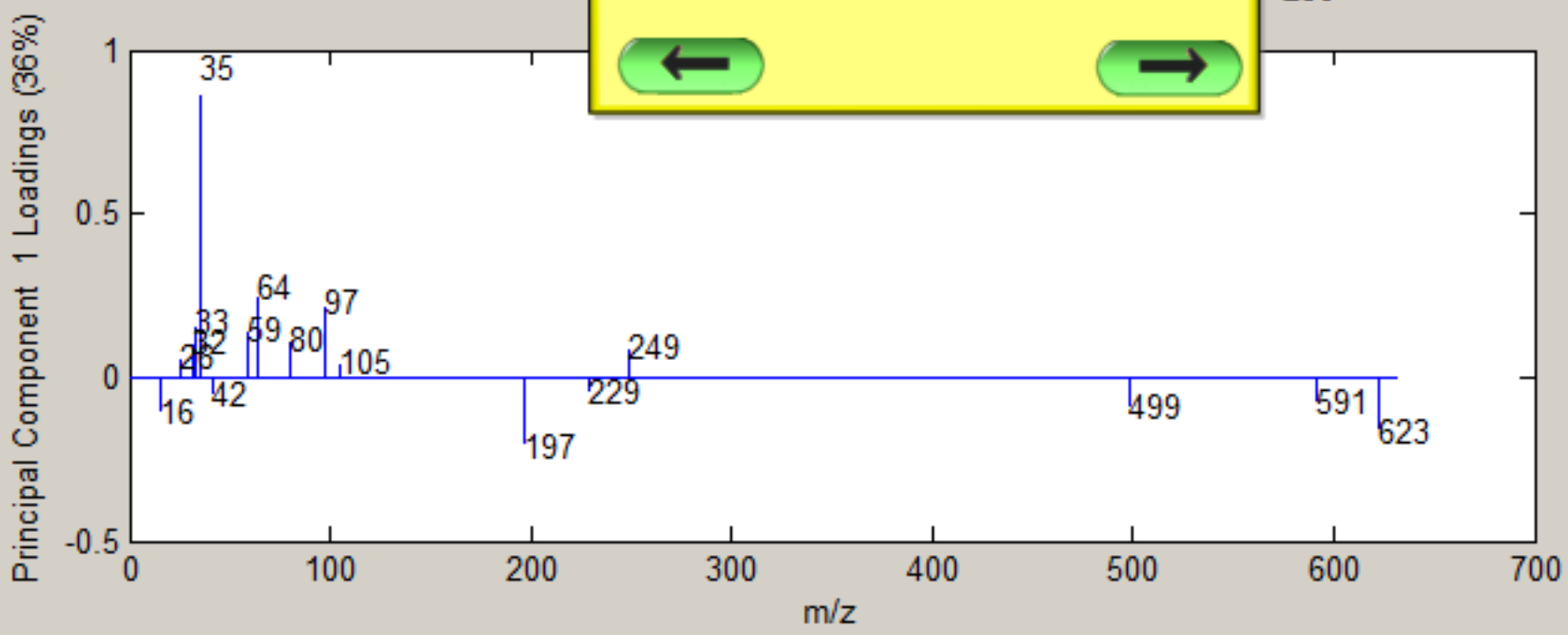
4 number PCs for Grid

Plot Multiple PCs in Grid

Opens a separate figure window




Then press the 'Plot Multiple PCs in Grid' button. A figure will open up in a separate window showing the requested score images.




Close Panel

imagegui

File Data Pre Processing MVA Data Display Image Processing

## Data Selection Panel

Name of Image Matrix: imagedata_DAN...

Name of Variable Matrix:

Load Selected

Image: imaged

Variables exactm

Data Preproces

PoissonScaling & Mean Cent

Run PCA

| PC# | %Var | PCA Summ %Var |
|---|---|---|
| 1 | 35.8 | |
| 2 | 6.1 | |
| 3 | 4.6 | |
| 4 | 3.8 | |
| 5 | 3.7 | |
| 6 | 3.6 | |
| 7 | 3.5 | |
| 8 | 3.5 | |
| 9 | 3.4 | |
| 10 | 3.4 | |

Name for scores

Name for loadings

Name for Variance

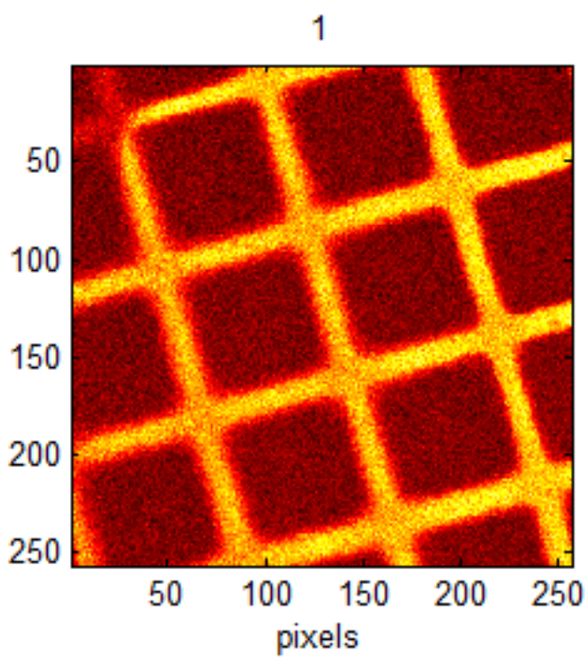
# of PCs to keep in model

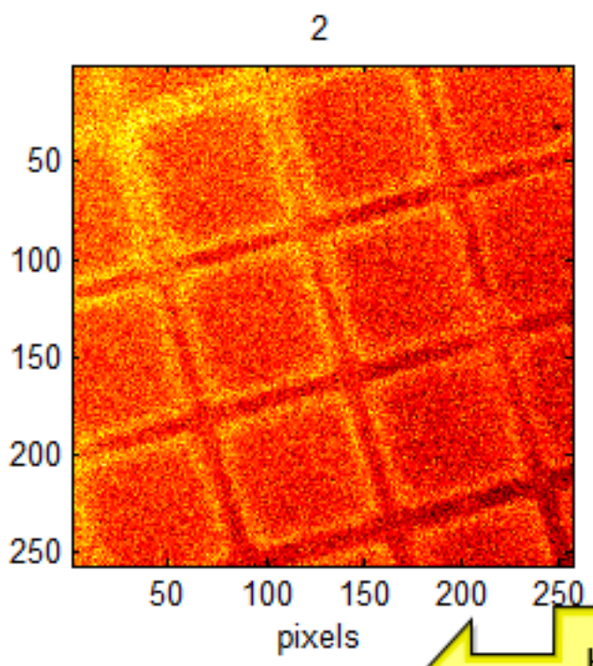
Save PCA Data

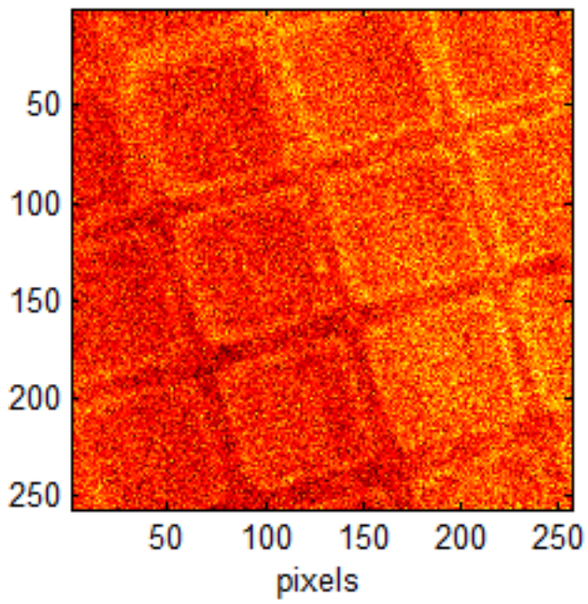
Close Panel

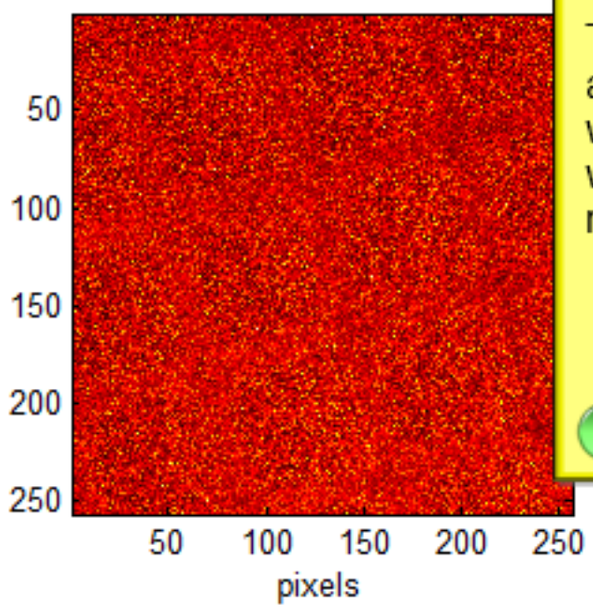
Figure 1

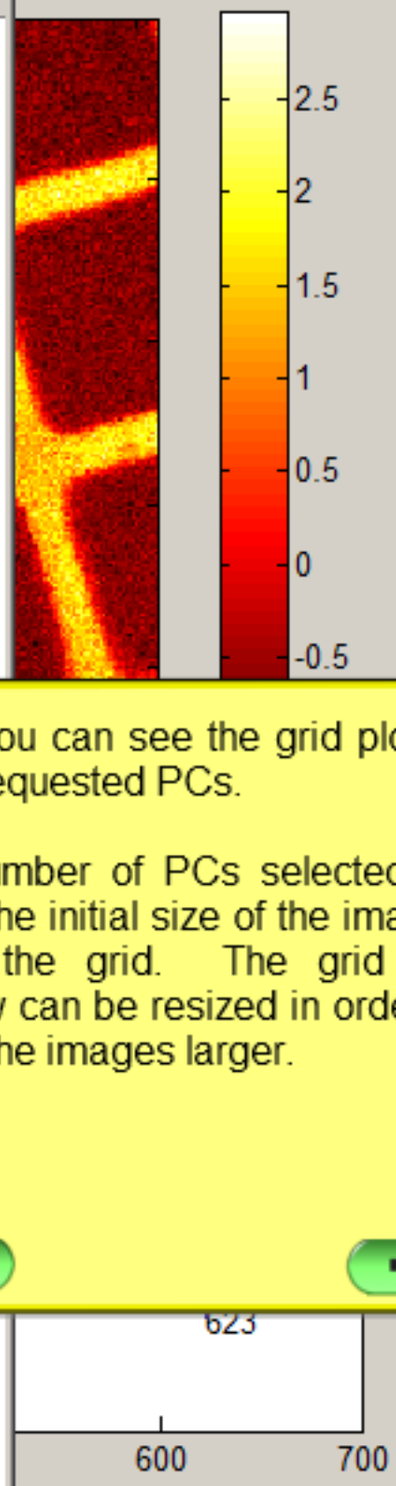
File Edit View Insert Tools Desktop Window Help




Here you can see the grid plot of the 4 requested PCs.

The number of PCs selected will affect the initial size of the images within the grid. The grid plot window can be resized in order to make the images larger.

imagegui

File  Data Pre Processing  MVA  Data Display  Image Processing

## Data Selection Panel

Name of Image Matrix: imagedata_DAN...

Name of Variable Matrix: exactmass_DAN01

Load Selected Data

Image: imagedata_DAN01

Variables: exactmass_DAN01

Data Preprocessing: Poisson Scaling & Mean Center

Run PCA

PCA Summary

| PC# | %Var | %Vartotal |
|---|---|---|
| 1 | 35.8 | 35.8 |
| 2 | 6.1 | 41.9 |
| 3 | 4.6 | 46.5 |
| 4 | 3.8 | 50.3 |
| 5 | 3.7 | 54 |
| 6 | 3.6 | 57.6 |
| 7 | 3.5 | 61.1 |
| 8 | 3.5 | 64.6 |
| 9 | 3.4 | 68 |
| 10 | 3.4 | 71.4 |

Name for scores matrix: scores

Name for loadings matrix: loads

Name for Variance matrix: var

# of PCs to keep in model: 4

Save PCA Data

PC #: 1

Plot Scores and Loads

Split Pos/Neg S&L

Opens a separate figure window

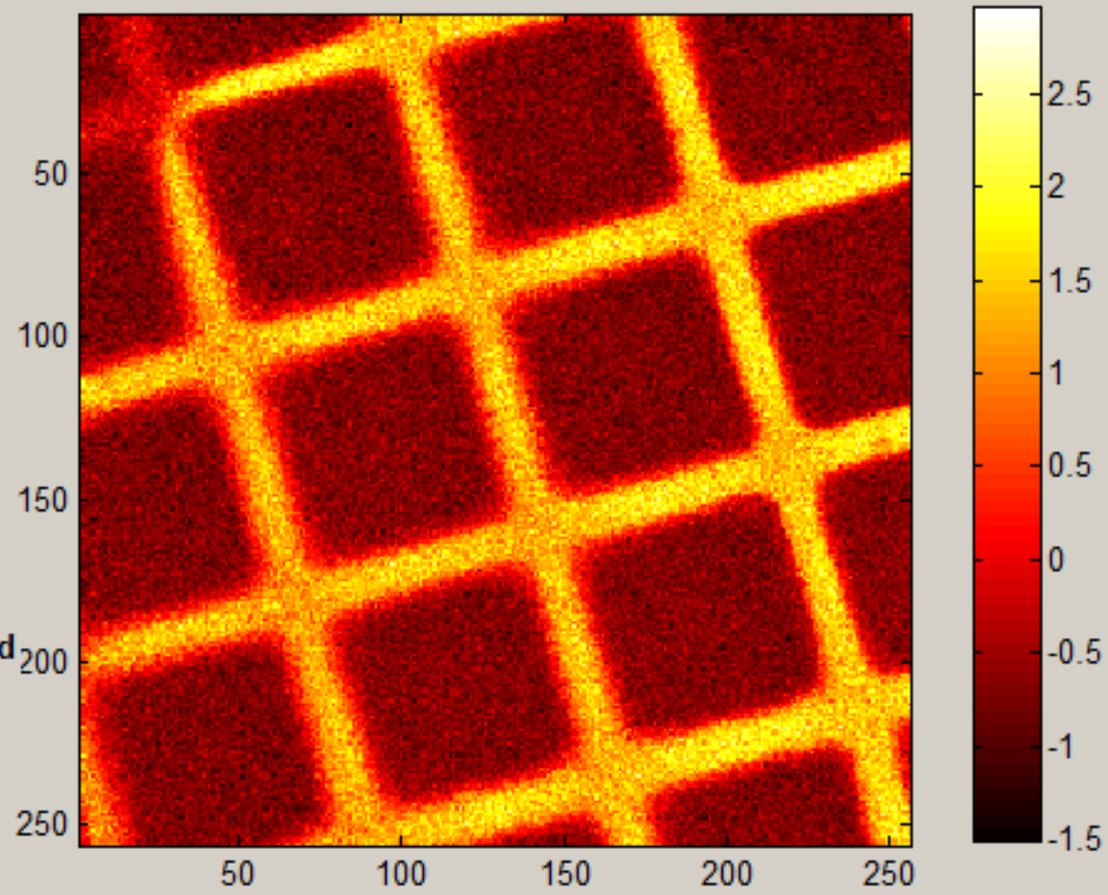
Browse all PCA plots

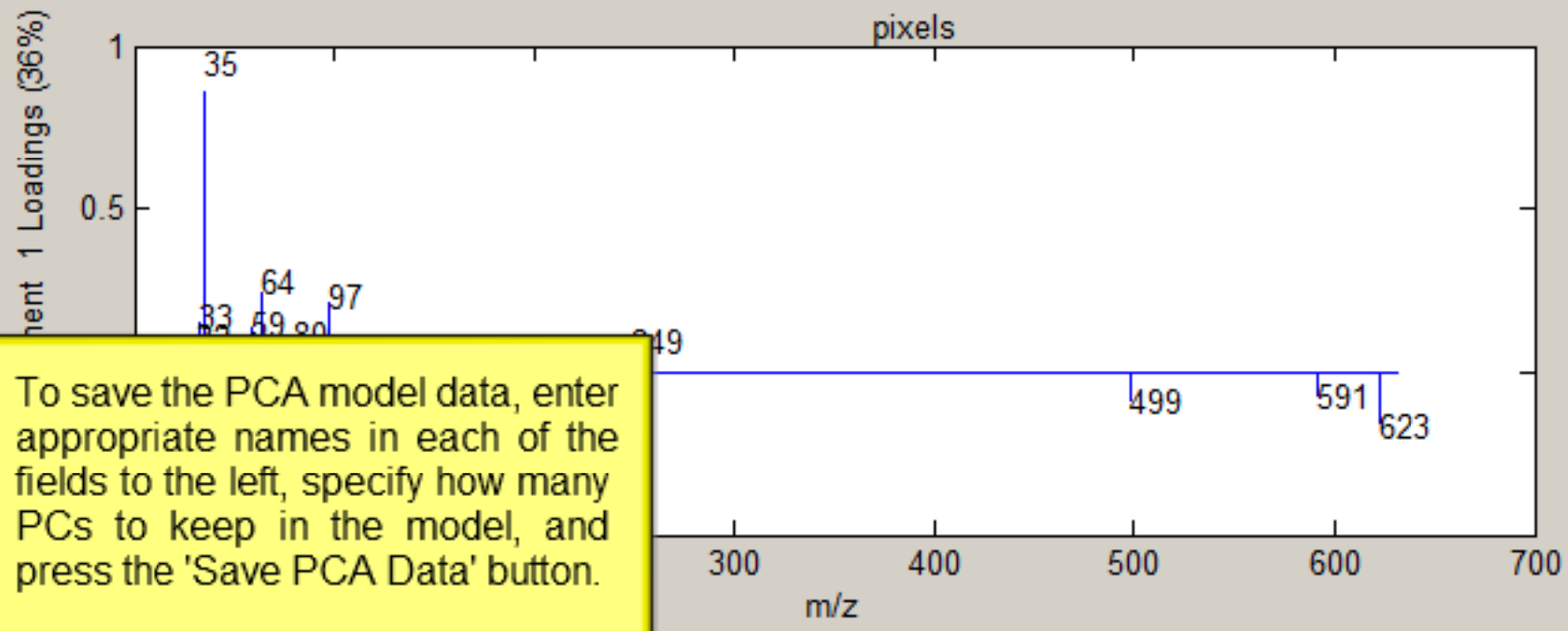
Opens a separate figure window

4 number PCs for Grid

Plot Multiple PCs in Grid

Opens a separate figure window




To save the PCA model data, enter appropriate names in each of the fields to the left, specify how many PCs to keep in the model, and press the 'Save PCA Data' button.

You must save the PCA model data in order to use the functions to plot the scores and loadings in the 'Data Display' menu.

Close Panel

imagegui

File  Data Pre Processing  MVA  Data Display  Image Processing

## Data Selection Panel

**Name of Image Matrix**: imagedata_DAN...

**Name of Variable Matrix**: exactmass_DAN01

Load Selected Data

**Image:** imagedata_DAN01

**Variables** exactmass_DAN01

**Data Preprocessing**

Poisson Scaling & Mean Center

Run PCA

**PCA Summary**

| PC# | %Var | %Vartotal |
|---|---|---|
| 1 | 35.8 | 35.8 |
| 2 | 6.1 | 41.9 |
| 3 | 4.6 | 46.5 |
| 4 | 3.8 | 50.3 |
| 5 | 3.7 | 54 |
| 6 | 3.6 | 57.6 |
| 7 | 3.5 | 61.1 |
| 8 | 3.5 | 64.6 |
| 9 | 3.4 | 68 |
| 10 | 3.4 | 71.4 |

**Name for scores matrix**: scores

**Name for loadings matrix**: loads

**Name for Variance matrix**: var

**# of PCs to keep in model**: 4

Save PCA Data

**PC #**: 1

Plot Scores and Loads

Split Pos/Neg S&L

Opens a separate figure window

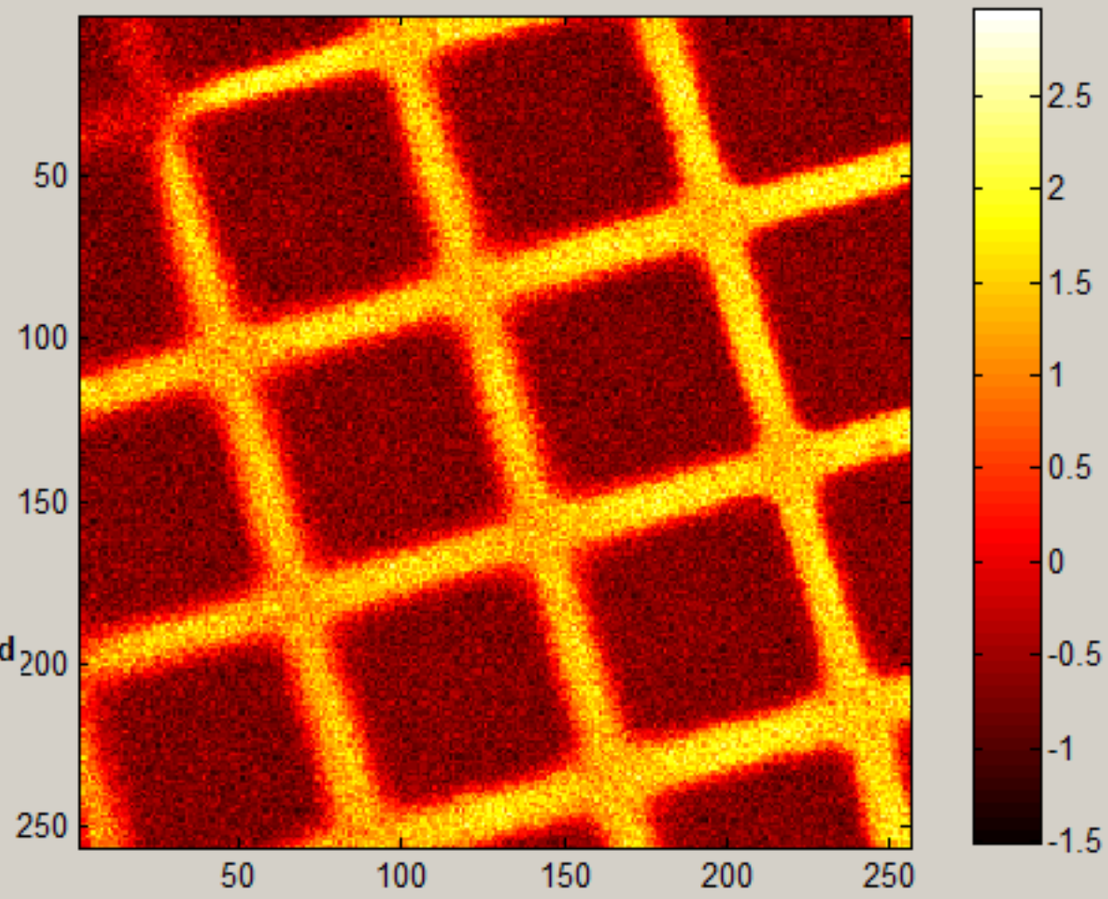
Browse all PCA plots

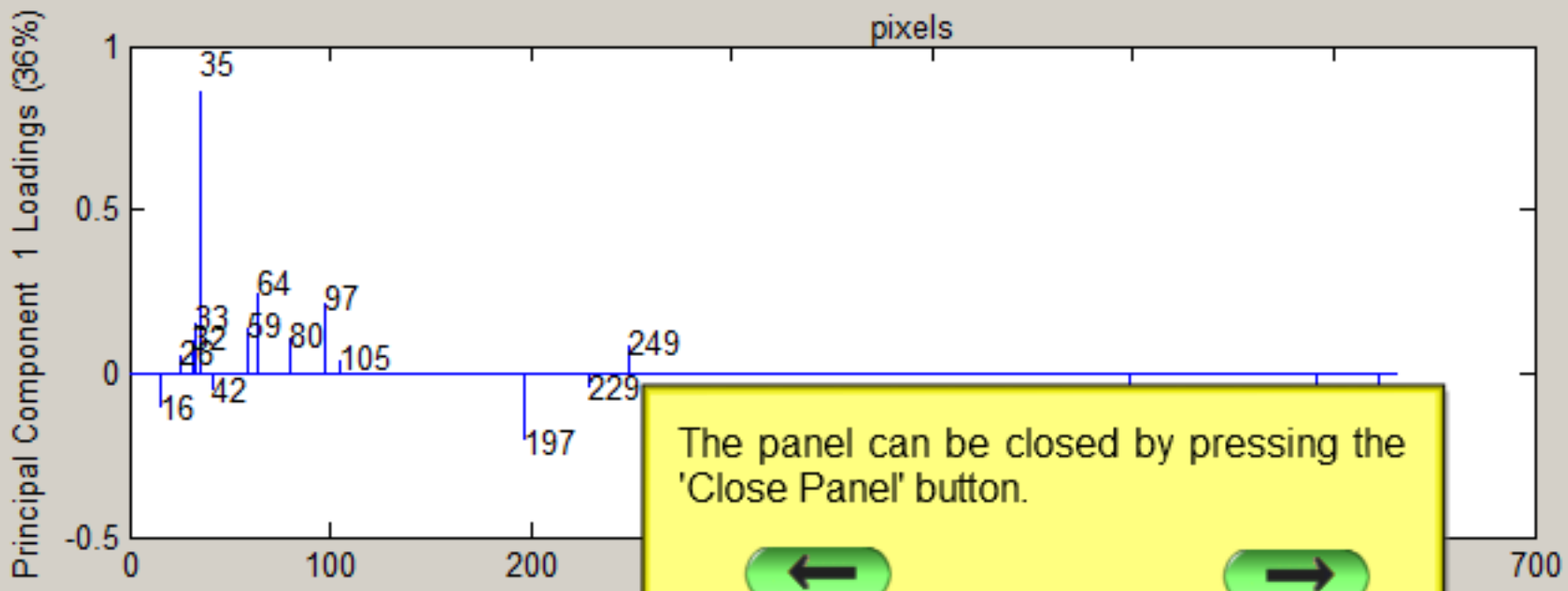
Opens a separate figure window

4 number PCs for Grid

Plot Multiple PCs in Grid

Opens a separate figure window




The panel can be closed by pressing the 'Close Panel' button.

Close Panel

imagegui

File Data Pre Processing MVA Data Display

**Data Selection Panel**

**Name of Image Matrix** imagedata_dan01

**Name of Variable Matrix** exactmass_dan01

That ends this tutorial. Press the button on the left to go back to the previous step. Press the button on the right to start the tutorial over.