

Notes on the use of Itools GUI

Conditions and warranty

ItoolsGUI is a freeware Gui (**G**raphical **U**ser **I**nterface) for the Itools toolbox by Lars Nørgaard and Riccardo Leardi available for download at <http://www.models.kvl.dk/source/>

No Guarantees are given for the quality of the GUI or the consequence of this use
The toolbox has been tested with Matlab 7.04 in Windows XP SP2. It seem to work fine also in Matlab 6.5 (excluding NipalsGUI)

Feel free to modify the GUI or implement new features. If you will do so I will be happy to know. If you have problem running the Gui contact me via email at giorgio.luciano@inwind.it . I will try to fix the problem.

Setting Up

Requirements are the same of ITOOLS toolbox

Just extract the content of the zip file under a directory and add it to your matlab pathfile

In order to make NipalsGUI you will have also to install autoscal.m and var.

Enjoy it ;)

Getting Started

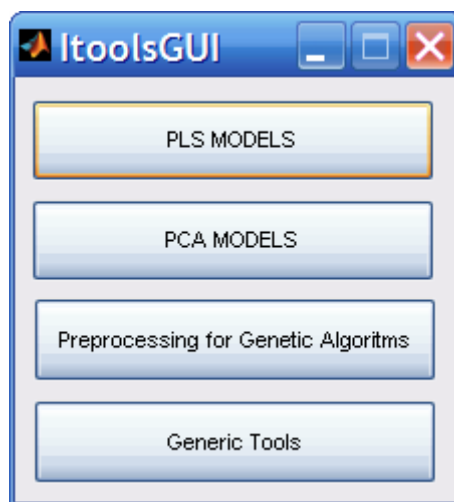
In this short “help” I will report examples of the use of the Gui, since it is of intuitive use. For an extended help about the function that it uses refers to the Itoolbox manuals.

Interval PLS

We will follow the example in the ITOOLS manuals.
Firs of all open the ItoolsGUI typing in the Matlab prompt

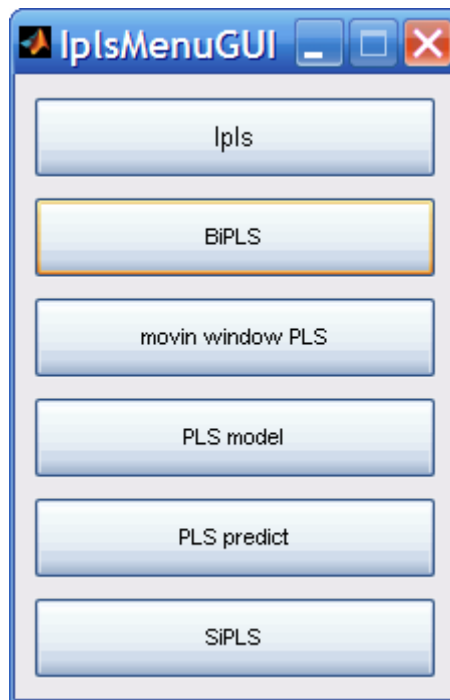
```
> ItoolsGUI
```

an Window Like this will open

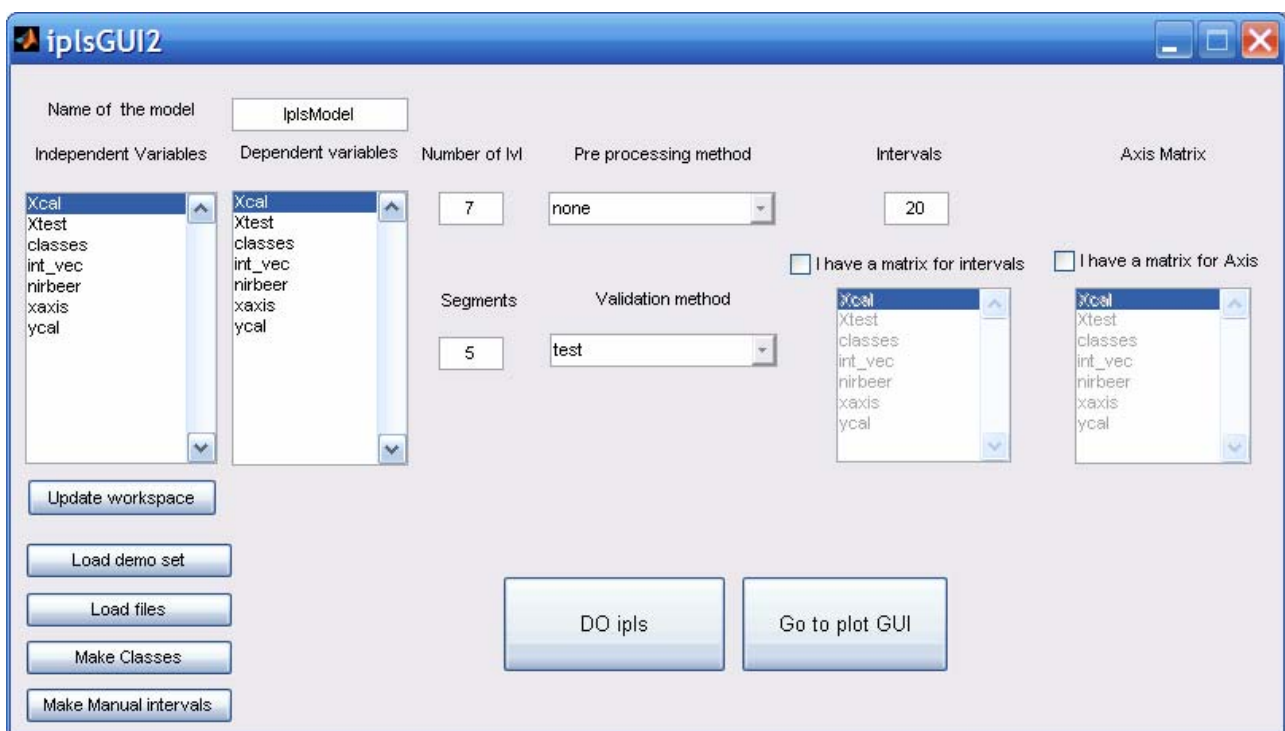


we choose **PLS models**

and another window will open



finally we want to perform a IPLS and so we choose **IPLS**



We want to open the demo set and so we click on **Load demo set**.

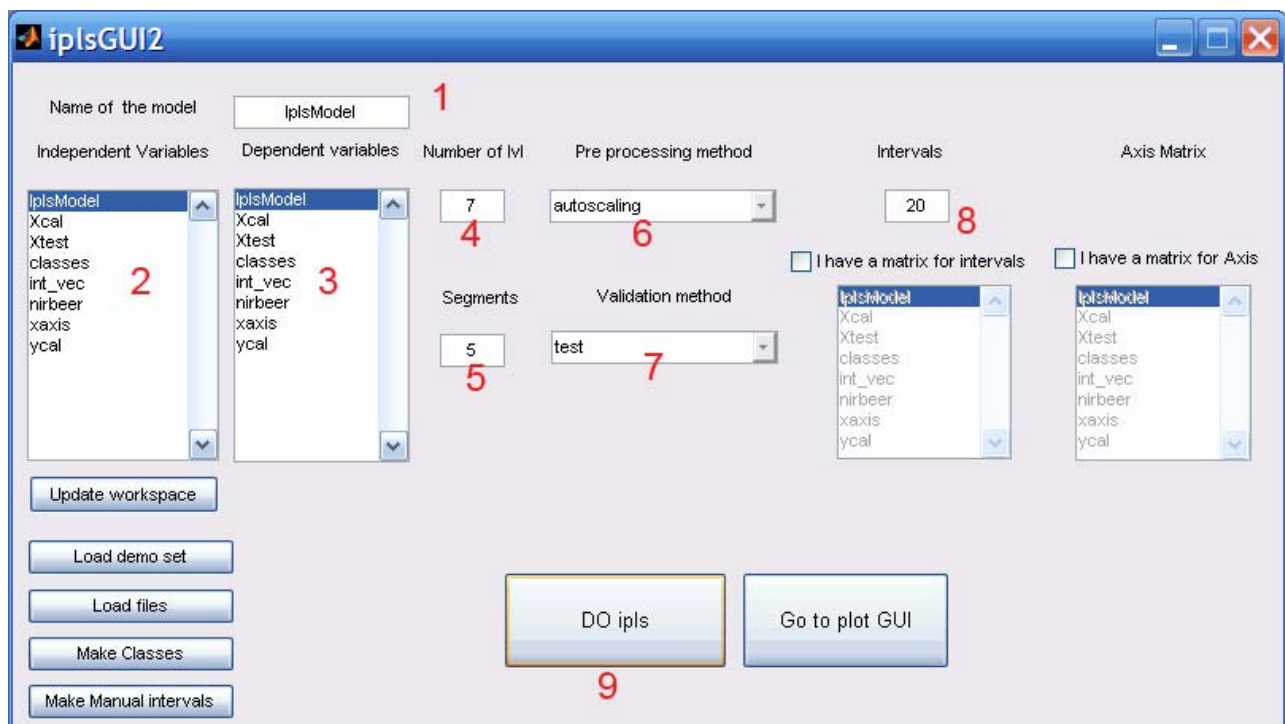
Click also on **Make classes** and **Make Manual Intervals**.

Now just notice that in your Matlab workspace we have everything we need.

If you want to open your own data just click on open file. Your data will be loaded as a structure.

We want to perform a PLS and so

- 1) first of all choose a name for your model (if you forget to do it don' worry, your model will have the default name of IplsModel)
- 2) choose the name of your X data matrix (click on it)
- 3) choose the name of you y matrix (just click on it)
- 4) type the number of level (default 7)
- 5) choose the number of segments (default 5)
- 6) choose the preprocessing method (default none)
- 7) choose validation method
- 8) choose the number of intervals (default 20) or if you have a vector for interval check the checkbox and choose you interval vector (if you have vector for axis check the axis checkbox and choose your vector matrix otherwise leave the checkbox unchecked)

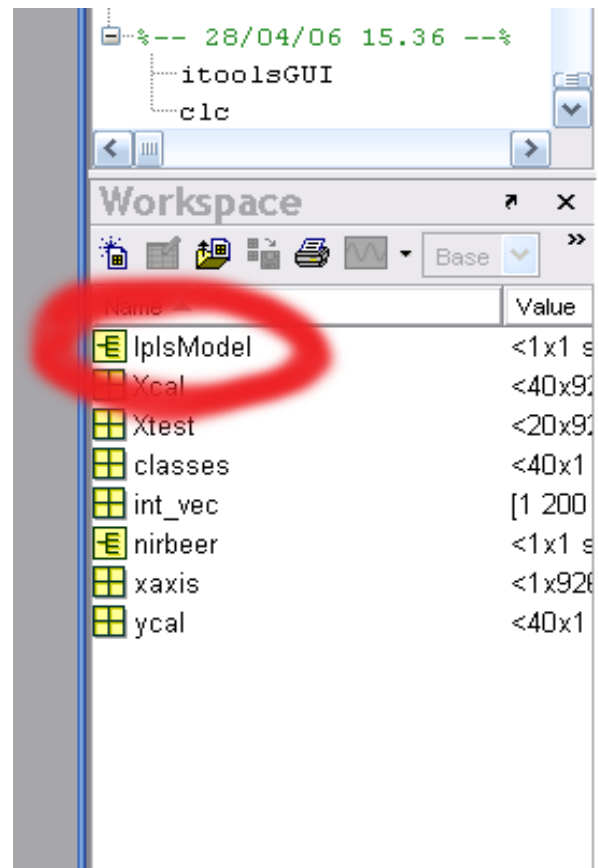


What you have done corresponds to writing in you matlab command line

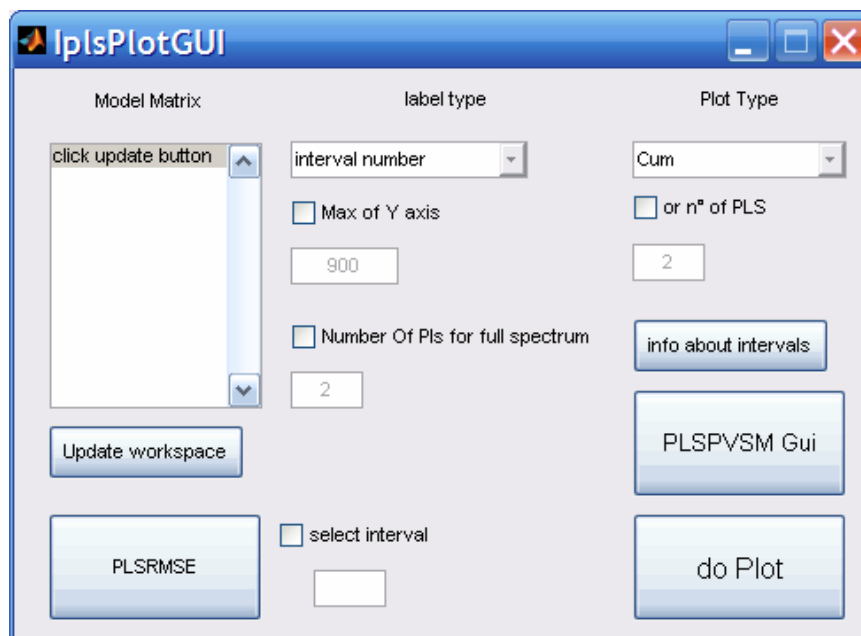
```
> Models=ipls(Xcal,ycal,10,'mean',20,axis,'syst123',5);
```

Now just click on **Do IPLS** and you're done.

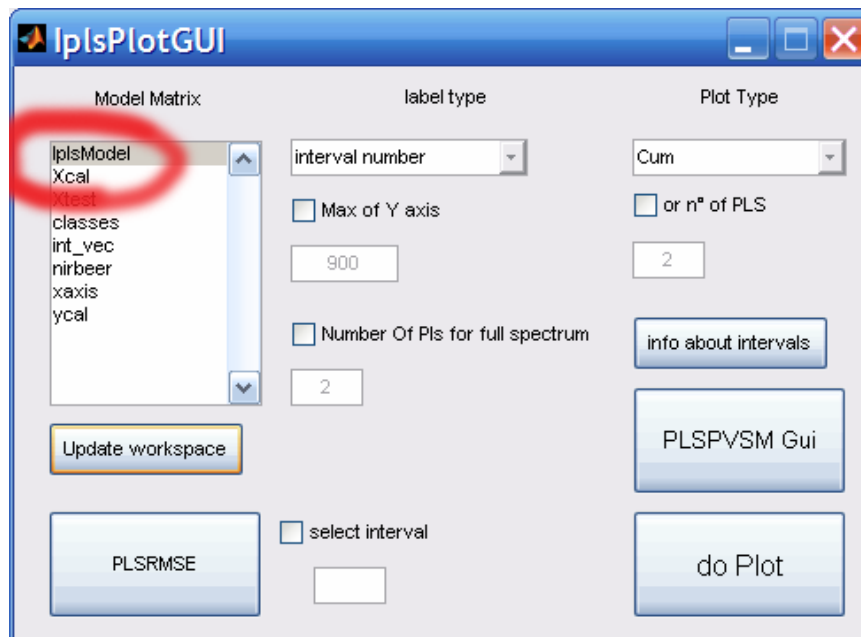
Have a look at the Matlab workspace and you will find your IPLS model.



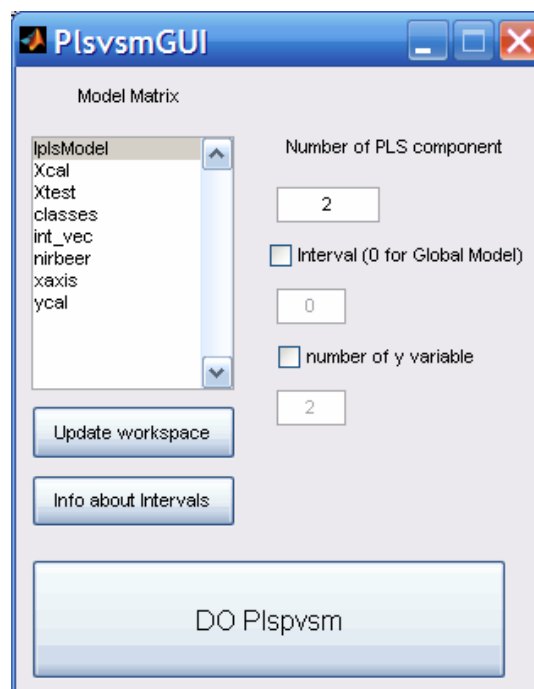
Now we need plot. So just click on **Go to plot GUI**.
This window will open



Push **Update Workspace** and you will see your model



Choose you model matrix and decide which kind of model you want
Clicking on PLSPVSM will open the GUI for plotting a Plspvsm



Other PLS models work in a similar way, just put the parameter in the mask and you will have yor model.

PCA

Ipca

Choose IPCA from the menu

A mask similar to that of Ipls will open (here we do not have a y matrix)

ipcaGUI

Name of the model: IpcaModel

Data Matrix: IpcaModel, Xcal, Xtest, classes, int_vec, nirbeer, xaxis, ycal

Number of PC: 7

Pre processing method: none, mean centering, autoscaling, MSC+mean centering, MSC+autoscaling

Number of Intervals: 20

Axis Matrix: IpcaModel, Xcal, Xtest, classes, int_vec, nirbeer, xaxis, ycal

Update workspace

Load demo set

Load files

Make Classes

Make Manual intervals

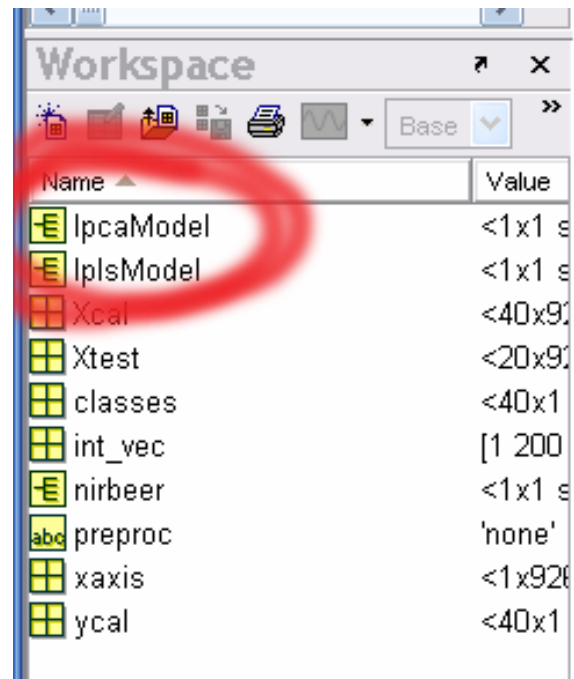
DO IPCA

Score Plot GUI

Load Plot GUI

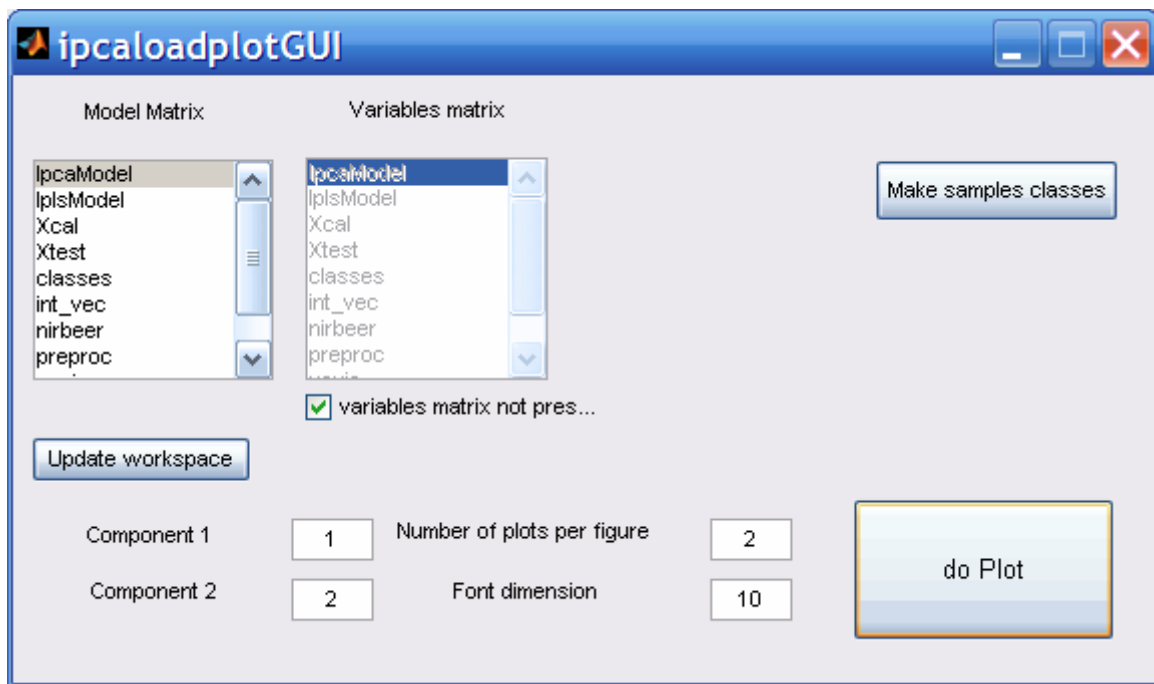
- 1) Choose the name for you Model (default IpcaModel)
- 2) Choose the name of your data matrix
- 3) Choose Number of Principal component
- 4) Preprocessing method
- 5) Number of intervals (or if you have a vector for your intervals check the checkbox and choose your matrix, you can do the same if you have an Axis matrix)
- 6) click on Do IPCA

Check you workspace and you will find your IPCA model



If you want Score Plot or Loadings Plot just click on **Score Plot GUI** of **Load Plot GUI**



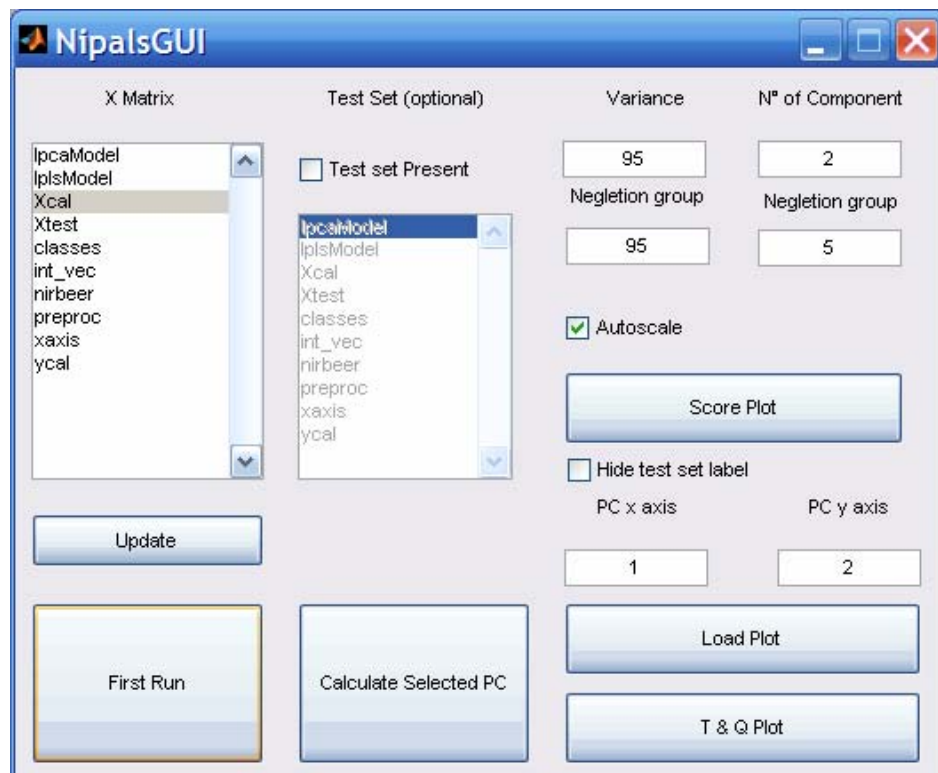


If you need more “custom” plots just go to generic **tools => 2d plot**

NipalsGUI can give a bit more information. It is the GUI for nipals made by riccardo Leardi based on Brereton Algorithm.

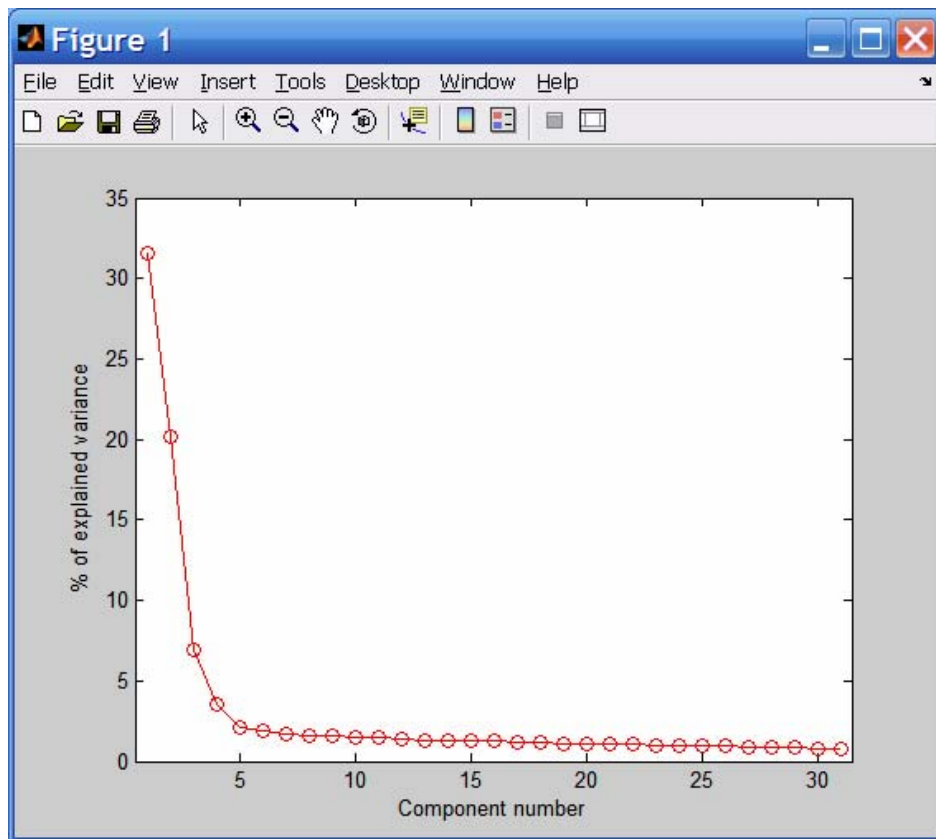
Let's see what we can do.

First of all just choose you matrix and then choose all other settings (if you use the demo set remember to check the autoscale checkbox otherwise you will obtain all variance in one component !)



Then click on **First Run**

A window like this should be open



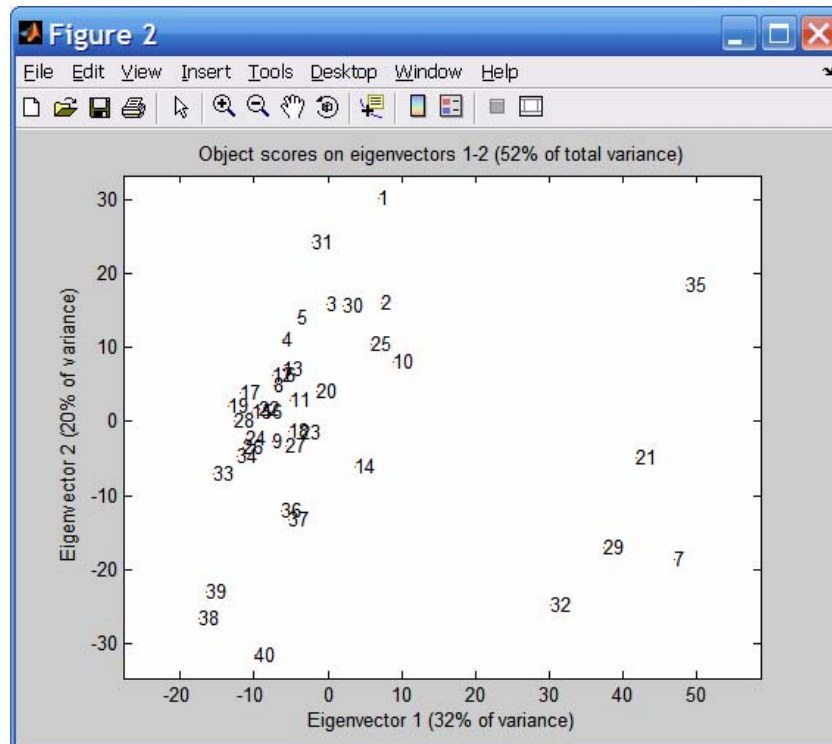
Here you can see the % of explained variance depending on how many component you will like to choose

So select how many component you would like to calculate and the click on **calculate selected PCs** (5 for example)

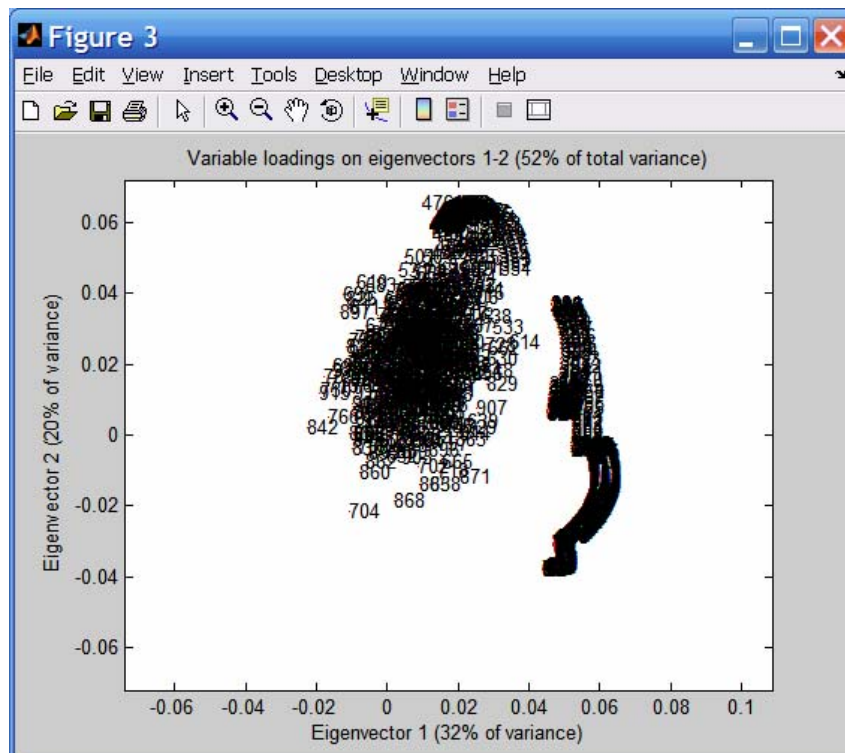
Name	Value
lpcaModel	<1x1 struct>
lplsModel	<1x1 struct>
Xcal	<40x926 double>
Xtest	<20x926 double>
classes	<40x1 double>
int_vec	[1 200 201 500 501 926]
lmat	<2x926 double>
nirbeer	<1x1 struct>
preproc	'none'
qcont	<40x926 double>
smat	<40x2 double>
tcont	<40x926 double>
xaxis	<1x926 double>
ycal	<40x1 double>

As you can see you workspace will be updated with all you matrices (score plot/ loadings plot etc etc) And now if you want plots, just click on the corresponding button For example

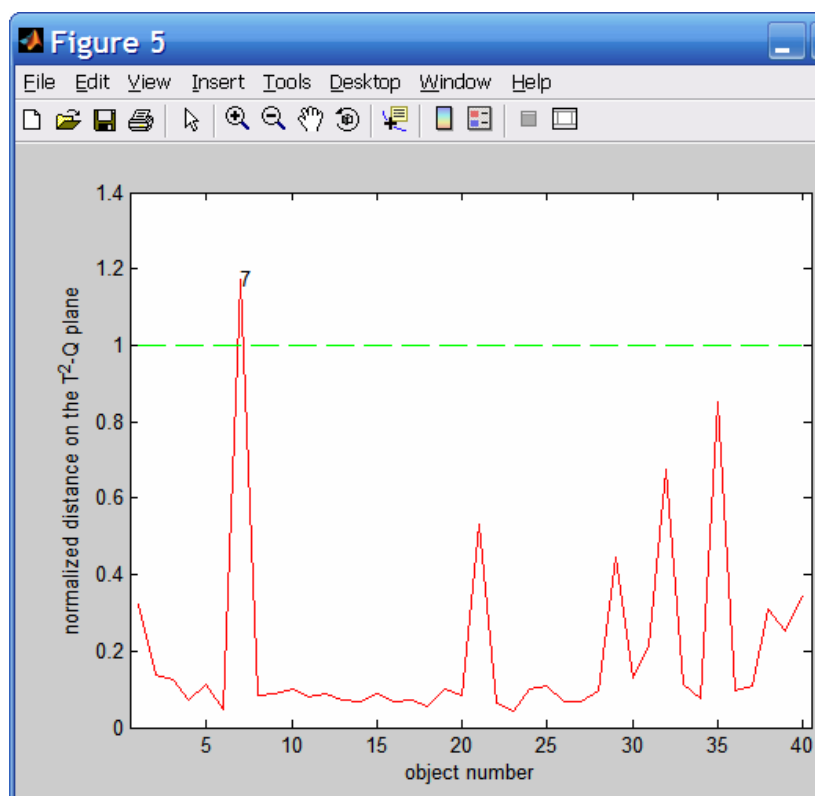
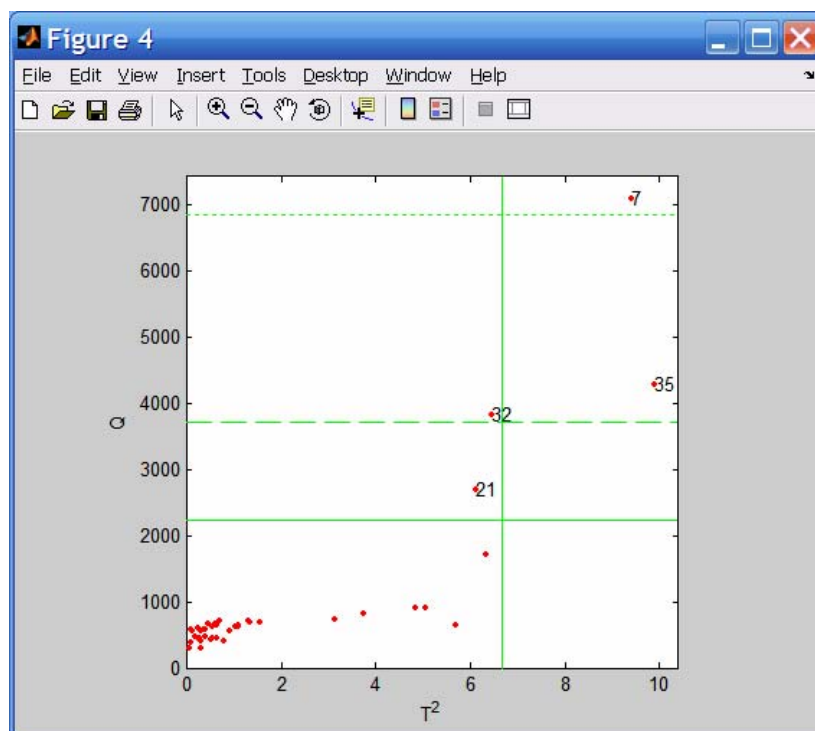
Score plot



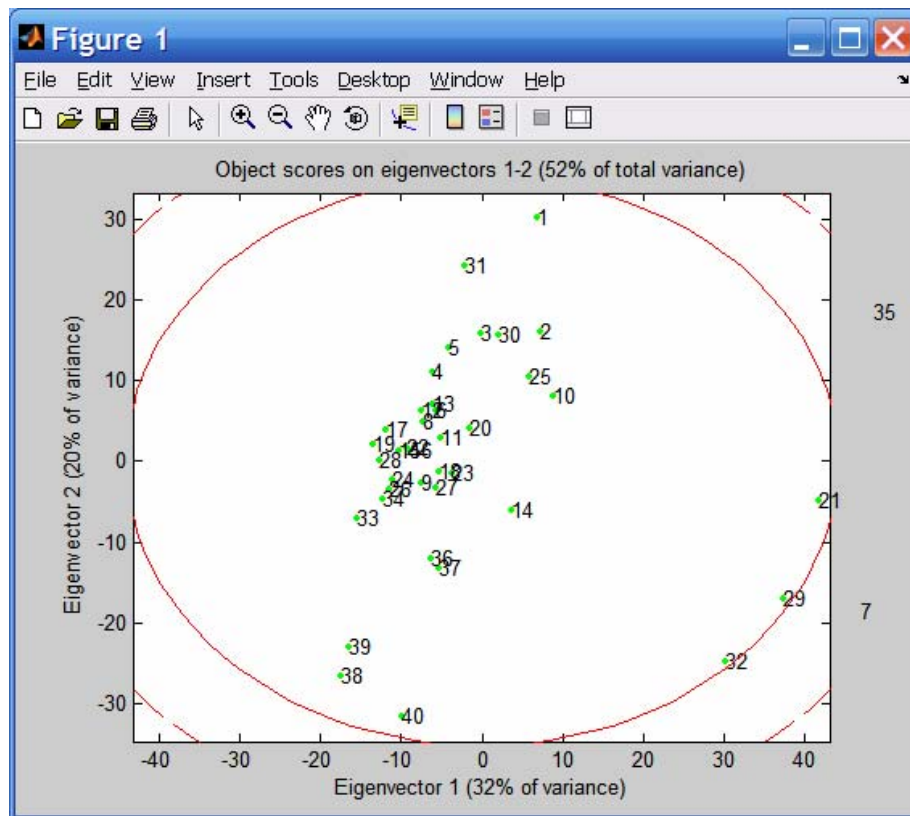
Loadings Plot



T and Q



If you have chosen a test set Nipals can give you also plots like this



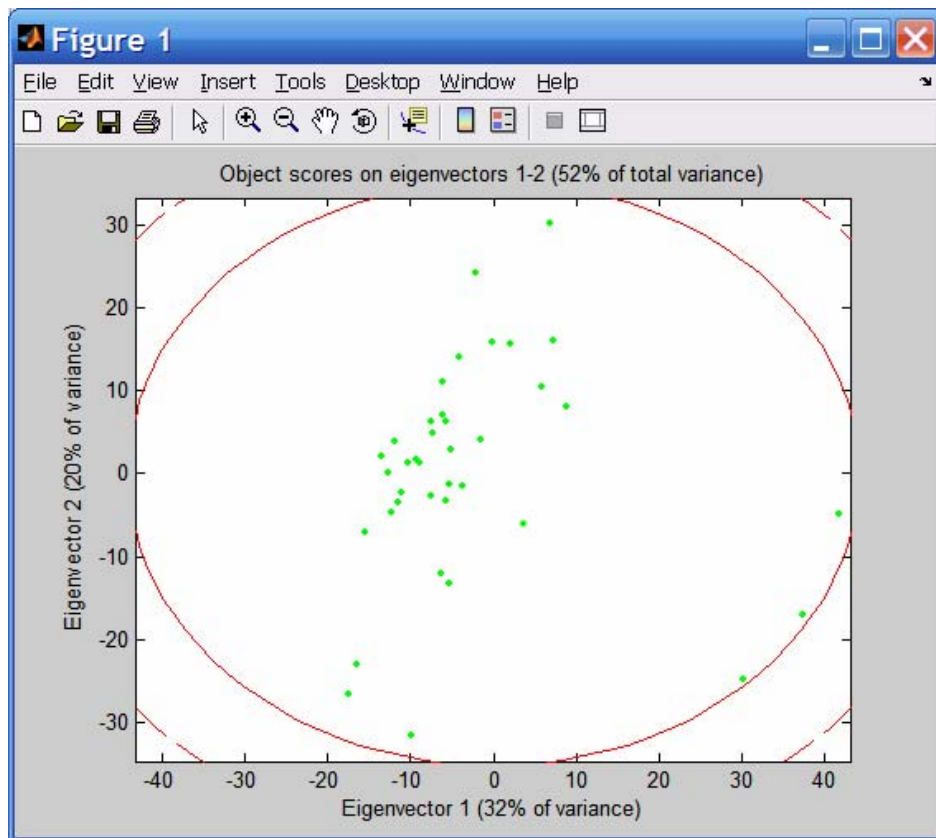
Or without test set label

NipalsGUI

X Matrix	Test Set (optional)	Variance	N° of Component
<ul style="list-style-type: none"> IpcaModel IpplsModel Xcal Xtest classes int_vec nirbeer preproc xaxis ycal 	<input checked="" type="checkbox"/> Test set Present	95 Neglection group	2 Neglection group
	<ul style="list-style-type: none"> IpcaModel IpplsModel Xcal Xtest classes int_vec nirbeer preproc xaxis ycal 	95	5

☒ Autoscale
☒ Hide test set label
 PC x axis: 1 PC y axis: 2

Buttons: Update, First Run, Calculate Selected PC, Score Plot, Load Plot, T & Q Plot



Generic 2d and 3d plot (examples)

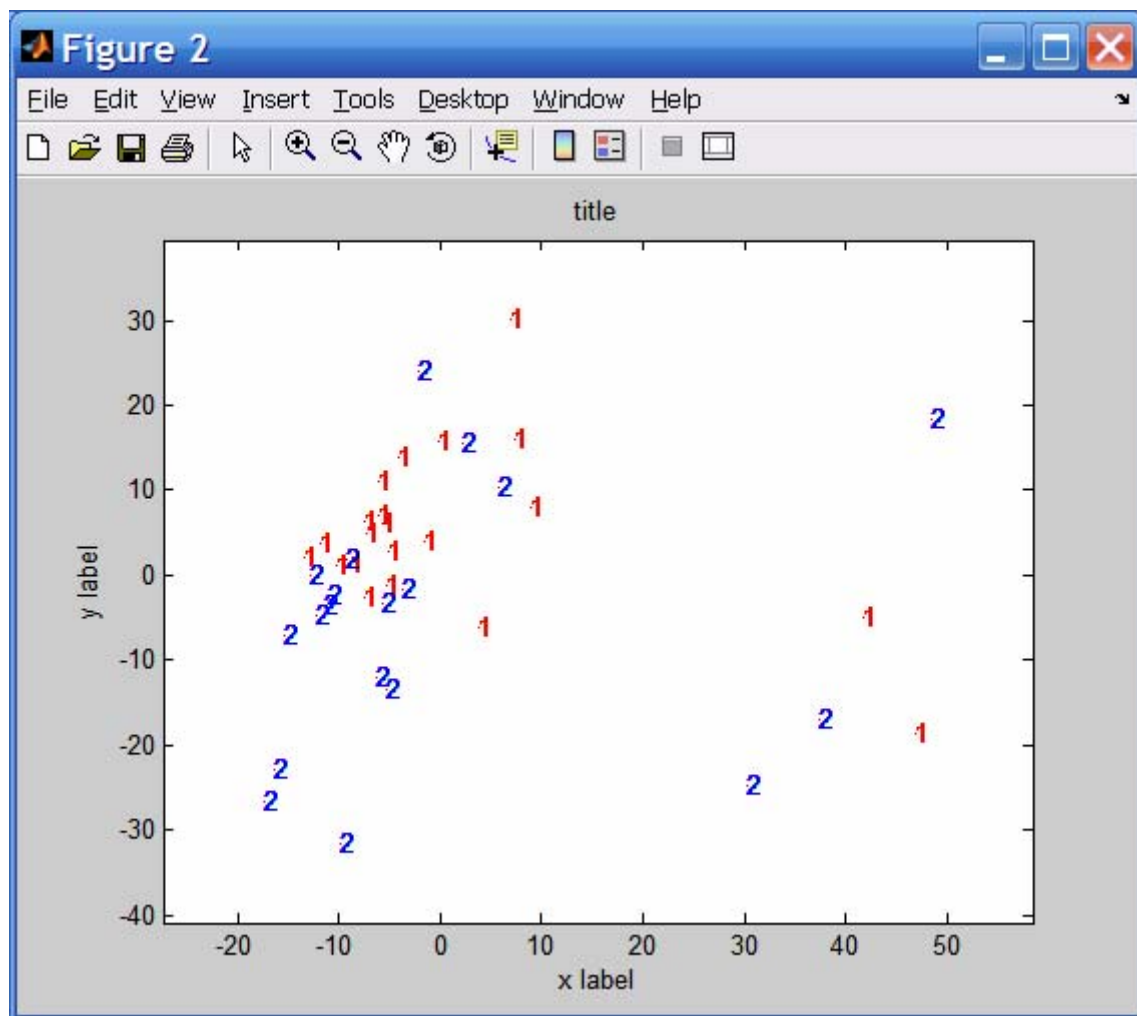
Plot2dGenericGUI

Matrix	Classes	Names	Xaxis	Y axis	X Label	Y Label	Title	Zoom x	Zoom y
lpcalModel lplsModel Xcal Xtest classes int_vec lmat nirbeer preproc qcont qcont2 smat	lpcalModel lplsModel Xcal Xtest classes int_vec lmat nirbeer preproc qcont qcont2 smat	lpcalModel lplsModel Xcal Xtest classes int_vec lmat nirbeer preproc qcont qcont2 smat	1	2	x label	y label	title	15	15

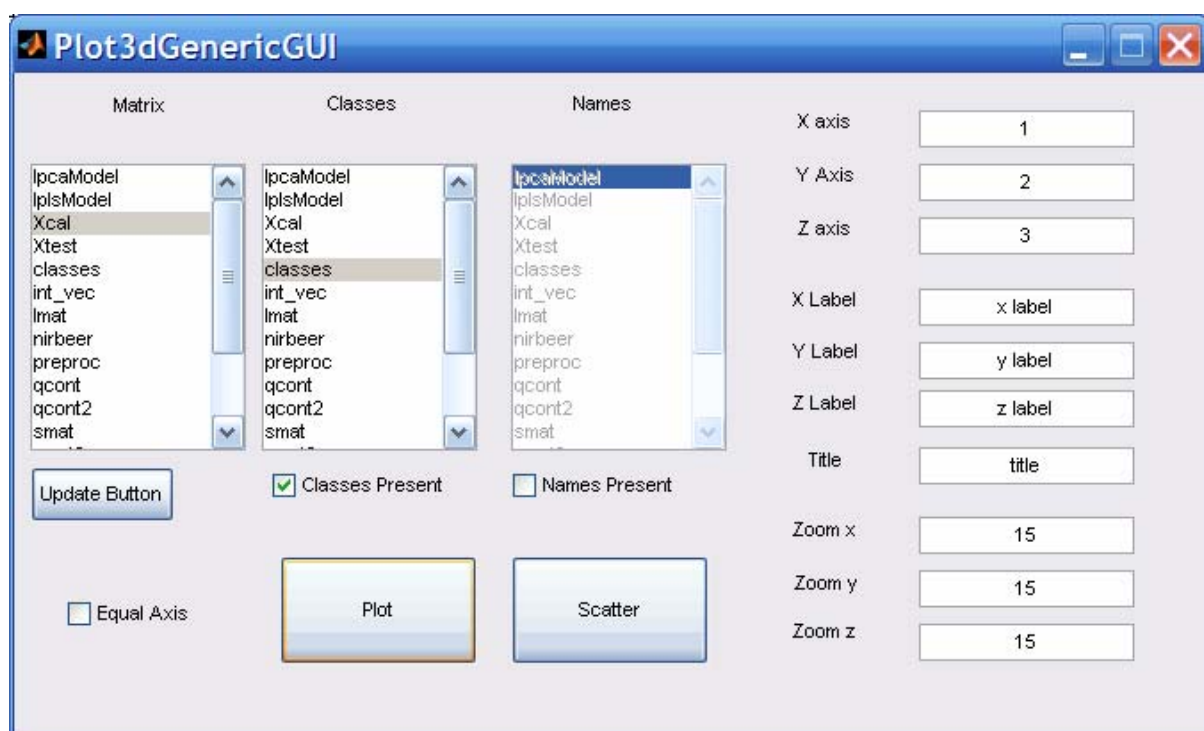
☒ Classes Present
 ☐ Names Present

☐ Equal Axis

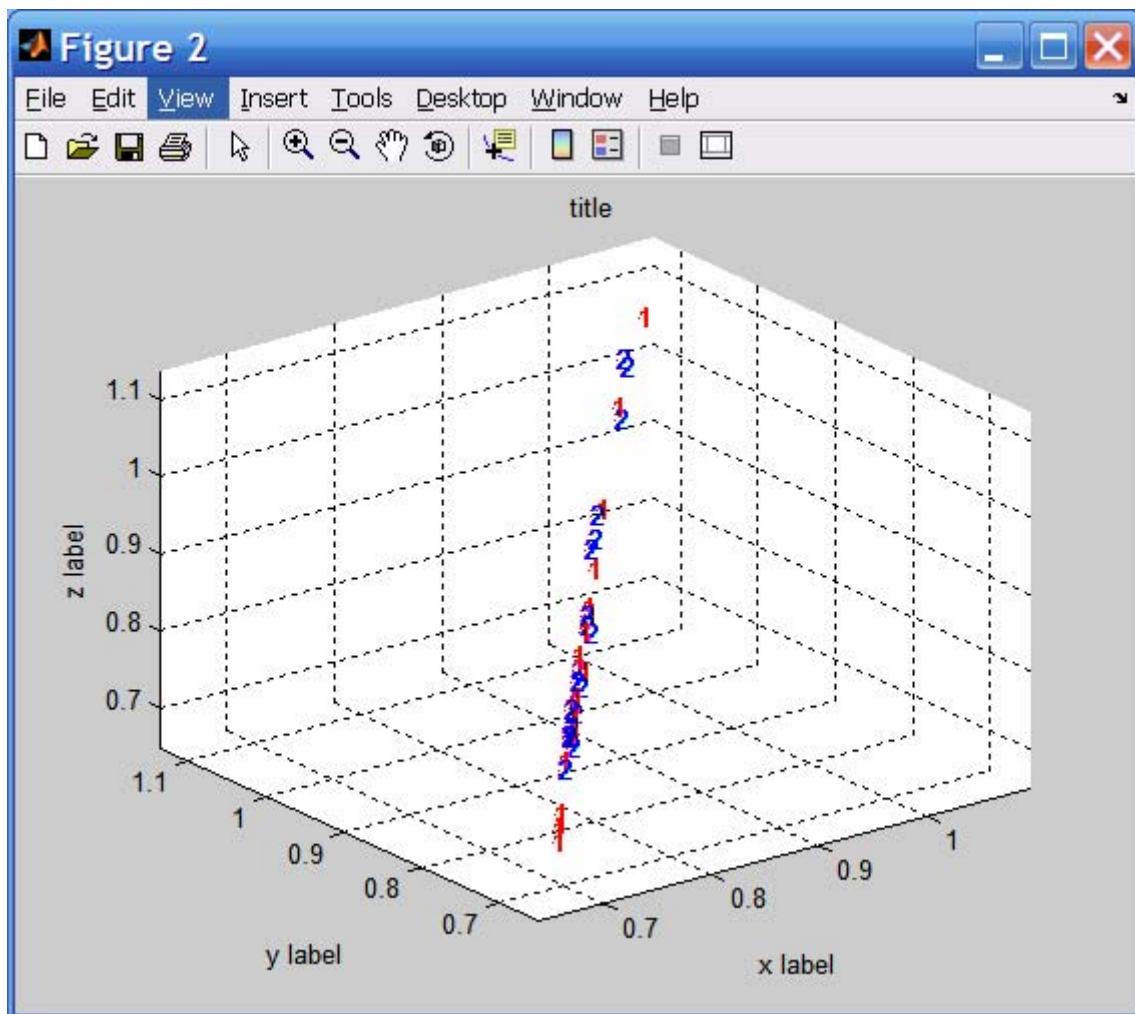
Generates



Or for 3d



Generates



2d and 3d plots incorporates a zoom function that can be useful when your point are “on the bound” of your axis.

They are simple interfaces for plot, scatter, gscatter, plot3 and scatter3 matlab commands. Just refer to matlab help for more details.