# ``xmgrace'' Power Spectrum Hints

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If you're not familiarwith xmgrace (aka qtgrace), then the following will help you get started in making a power spectrum. Note that in xmgrace, what is really computed in the amplitude spectrum (= square root of the power spectrum), but usually this is fine since we don't often care about the y-axis scaling.

Fire up xmgrace, then do the following:

i) Click on "Data" at the top, then → Import → ASCII
the find the directory where your file is located, then double click on it to load it in – or –
highlight the file and click "OK" at the bottom. Then click ``Cancel'' to exit and bring you back to the main plotting window.
(Note: if you are using the linx command line, just type:
 linux> xmgrace filename
and it will read in and plot the file.)

ii) To create the power spectrum, click on Data → Transformations → Fourier Transfrorm.
A new window appears, and the file you previously read in should be listed at the top as file S0.
If it is not highlighted, click on it.
Then select ``Let result X = frequency'' and at the bottom click DFT.
A new file will appear called S1 in the list. Click Close.
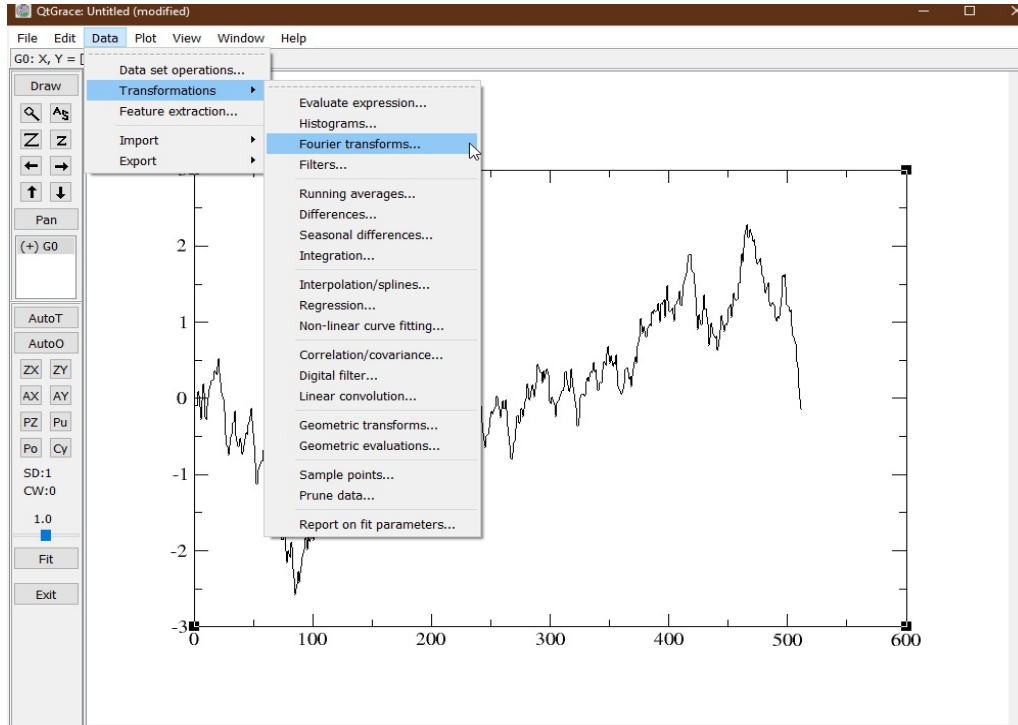
iii) Back in the main window, double click on the plotted data. A "Set Appearance" window will pop up. Right click on the top file (G0.S0) and in the pull-down menu that appears, click "Hide". The data file will vanish from the graph. Then right click on the G0.S1 file and click "Show. Click on Close to exit.
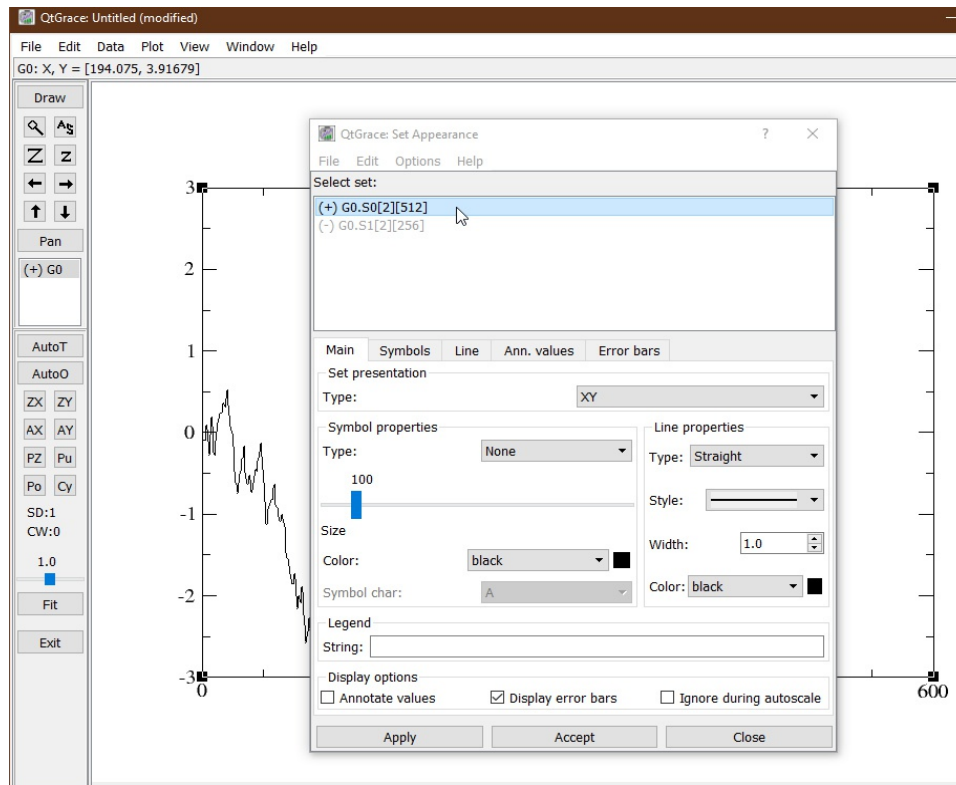
At this point it may look like nothing is there, but that's because the axis scales are completely wrong and need to be re-set. Click on the "AS" button on the top left to "AutoScale". You should now see your amplitude spectrum.

iv) To make pretty:
Click on the data curve to adjust color, thickness, drawing points, point size, etc.
Click on numbers along the y-axis to bring up a window to adjust the scales and enter labels.
Click at the top where the title should be to enter a title.
You always need to click "Apply" for the change to take effect.

v) To print, select File at the upper left, → Print setup (or file export setp) and take it from there.
vi) To save your xmgrace file, select File at the upper left → Save as, etc.
vii) To save (export) any of the data files to a file, activate the desired graph, select Data at the top menu → Export → ASCII then highlight the data set you want save in the Graph box (e.g. G0.S1). Enter filename in Selection box at the bottom and click OK.. The xmgrace filename should have the suffix ".agr", e.g. "HW5_sine.agr"

For a more informative figure, you can make a 2-panel plot so you can see the time series and its power spectrum on the same figure.

Start xmgrace, then

i) Click on Edit → then Arrange Graphs → select 2 Rows in Matrix → Apply → Close

ii) Data → Import → ASCII → load in data, then Cancel to exit

iii) Data → Transformations → Fourier Transfrom → ``Let result X = frequency" → DFT → Close

iv) Edit → Set operations →
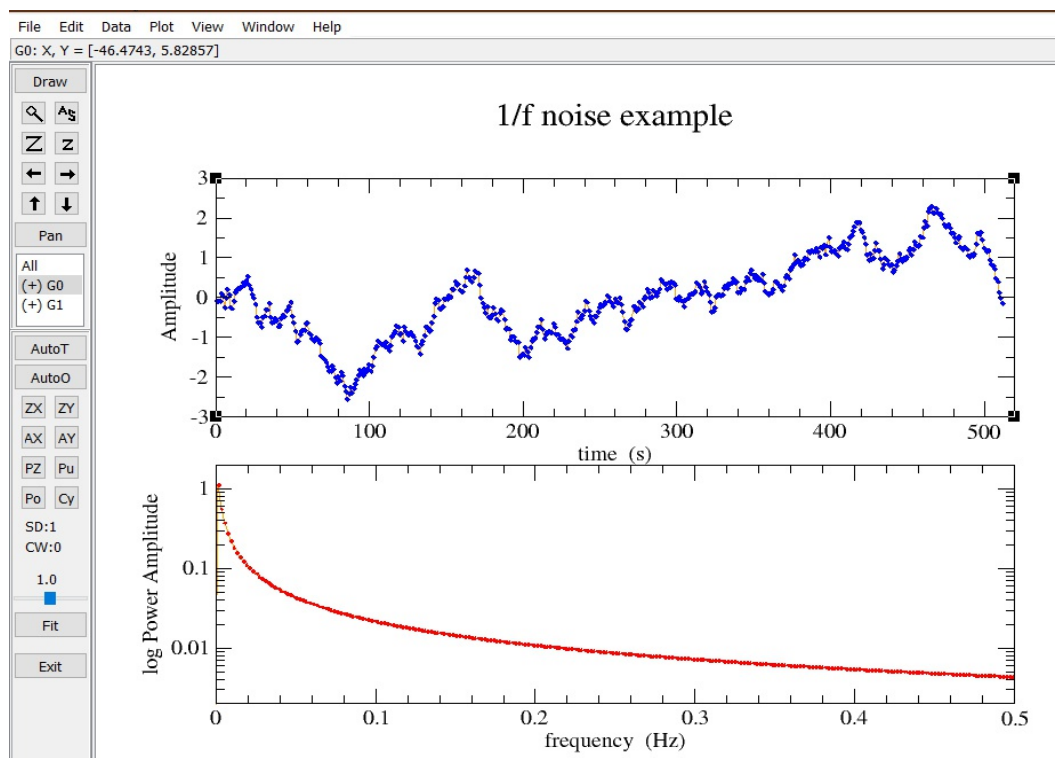   In Source Column (on the left top), highlight Graph G0
   In Source Set (on the left, highlight G0.S1
   In Destination Column (top right), highlight Graph G1
  Type of Operation: select Move in the pull-down menu
 Apply → Close
Click "AS" to autoscale.

Note: Now that there are two graphs, it can be confusing to edit things. What you need to do is pay attention to which graph is "activated". Notice the black boxes in the corners of the graph – that tells you which graph is activated.
To activate a graph (top or bottom), just click on (inside) the graph. Once activated, the usual xmgrace commands like zoom and labelling will work, but for that graph only.