GUI User Guide

Installation

To install the GUI, first download the repository off of GitHub. Once downloaded, enter the directory of the folder containing it and run the command "pip install -r requirements.txt" (you may need to replace "pip" with "pip3" depending on your OS). This will install all the packages needed to run the GUI. For this to work properly, you will need to have the program R installed on your computer, as well as the package JAGS.

Running the GUI

To run the GUI, first enter the directory of the folder containing it. Once you have entered this directory, run the file called "Spectrum_GUI.py".

File loading

To start analyzing a spectrum, press the button labeled "File" in the top left corner and subsequently select the "Load Spectrum File" button. This will bring up your computer's file menu screen, from which you can select the file that contains your desired spectrum. Once the file has been loaded, you're ready to start analyzing.

Zooming

To zoom in on a particular peak, from the toolbar (the strip of icons across the top of the GUI), select the magnifying glass icon that contains a plus sign in the center of it. This will convert your cursor into a cross-hair, with which you can click around the peak you want to zoom in on. A blue region will be created after your first click, which serves as a visual aid to highlight the region you are currently selecting. Once you click a second time, it will automatically zoom in on the region you selected. For precise control over the size of the viewing region, the arrows directly beside the zoom icon allow for you to expand (in the case of the up arrow) and contract (in the case of the down arrow) the viewing region by 15%. The slider at the bottom of the screen allow for you to move the region around, and you can select the icon labeled "Set full Y-Scale" to automatically adjust the y-scale to match the height of the largest channel in your current viewing region.

Peak and background selection

To actually start analyzing a specific peak in your spectrum, select the icon in the toolbar resembling a mountain with a flag sticking out of the top. Similar to the zooming mechanic, this option lets you click around the peak you want to study, with a light blue region showing the peak you've selected.

For more robust peak analysis that takes background into consideration, after you've chosen your desired peak you would then need to select the icon located directly to the right of the peak selection icon. The process of selecting the background is exactly the same as selecting the peak: use your first two clicks to select the first background region, and the next two for the second background region. This time, it will be a red region shwoing the area you have selected.

Peak analysis methods

For a simple summation that will give you the total number of counts contained in your selected peak, select the icon labeled "F". This can be done with or without any background regions selected.

The other summation methods do require background regions to be selected prior to using them, and are represented by the icons to the right of the "F" icon. The "MC" icon utilizes a summation method that is similar to the "F" option, but uses a Monte Carlo simulation to repeat the process a specified number of times, each time using randomly drawn channels from your selected background regions. The "B" icon uses an Markov Chain Monte Carlo (MCMC) algorithm to generate a probability density based on a Bayesian model. The GUI draws from that probability density to get the net count and centroid estimates. The black die icon located to the right of the Bayesian method is used to see where a certain value lies within this probability density (for the purposes of determining upper limits), and thus can only be used after using the "B" summation method.

The second-to-last icon, which is shaped like a Gaussian curve, is a Gaussian-fitting method. It again uses a MCMC algorithm, with this time the output being the parameters for a Gaussian that best model the peak you have selected. The mean of this Gaussian is the centroid, while integrating it gives us the net counts.

For both the Bayesian and Gaussian fitting summation methods, you will need to input parameters for the number of samples, the "burn-in" size (i.e, the number of samples that will be used to tune the algorithm) and the number of chains. The Gaussian fitting method also allows for you to input information about the sigma of the fitted Gaussian's if desired.

After you perform a summation method, you can clear the colored regions in several different ways. If you want to perform another summation method using the exact same background and peak region you just used, simply hit the icon corresponding to the summation method you just performed, and this will result in the peak and background regions reappearing where you last put them. If you want to change the background regions after performing a summation, press the background icon and it place the peak region where it was previously and allow you to select new background regions exactly as you did before. If you want to change both the peak and background regions, then you can select either the peak selection icon, or the refresh button (this is the icon with the arrows that form a circle).

Test data

The final icon, labeled "Test", is used to generate artificial data. This can be used to create spectra whose net count and centroid values are exactly known, and is useful for testing the validity of the GUI's summation methods. The spectrum file labeled "testing" is what contains the test data you generate, and is what should be loaded if you want to analyze it. "Sample size" is the number of counts used to create the peak, "location of peak" determines the peak's centroid, and "width of Gaussian" sets the spread of the count distribution.

Other features

The very first icon in the toolbar is simply an exit button, with the icon located beside it serving as a refresh button that will clear your viewing screen. An icon labeled "log" allows for you to convert the y-axis of the spectra plot into log-scale, with a second click converting it back to a linear scale. The bar on the left side of the GUI displays the spectra files you have previously opened, and by double-clicking an entry in this list it will re-open that file and display it. The button located at the bottom of this side-bar allows for you to clear its contents in the event it gets cluttered.

If you want to calibrate the energy of the channels, simply enter the slope and intercept corresponding to your detector and press the "Calibrate Energy" button, and the GUI will then display the energy associated with the channel your mouse is on at any given moment.

Key Shortcuts

The GUI has keyboard shortcuts implemented to make using certain features easier and more efficient.

Open file	Ctrl+O
Save file	Ctrl+S
Open "about" window	Ctrl+A
Exit GUI	Ctrl+Q
Refresh GUI	Ctrl+R
Zoom in	Ctrl+Z
Zoom out	Ctrl+Shift+Z
Expand window	Ctrl+Up
Contract window	Ctrl+Down
Open peak select tool	Ctrl+P
Open background select tool	Ctrl+B
Perform frequentist sum	Ctrl+F
Perform bayesian sum	Ctrl+Shift+B
Perform gaussian fitting	Ctrl+G
Perform double gaussian fitting	Ctrl+Shift+G
Convert to log scale	Ctrl+L
Open test data window	Ctrl+T
Open test data 2 window	Ctrl+Shift+T