The Plot-Add-Multiply Program

Matthew Marcus

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I. Introduction

This program has two basic functions, symbolized by the two tabs on its front panel. The first is that it reads one or more 2-column (Y vs. X) data files and plots them on the same scale. The color, line style, point style, etc. are adjustable using the standard graph tools provided by LabVIEW.

The second function is that it computes weighted sums or products of data:

$$Y(x) = \sum w_i y_i(x) \tag{1}$$

or

$$Y(x) = \prod y_i(x)^{w_i} \tag{2}$$

with the individual data files being viewed as tabulations of functions $y_i(x)$. The files are spline-interpolated to the grid provided by the first file and pruned to the interval in x overlapped by all files.

II. Plotting

The front panel in plot mode is shown in Figure 1. When you invoke the program, the file path indicators on the left and the plot on the right are both blank. Use the browse buttons on the file paths or fill them in manually to select which files are to be included. The files will then plot on the graph. By default, the graph is not autoscaled, so use the scaling buttons on the graph to get the data to plot on scale. See the manual <u>Common LabVIEW Conventions</u> if you don't know about LabVIEW graph tools.

The white buttons which are shown checked (with `X`'s) determine which files will be included in the plot. Check or un-check them to show or hide different curves. Note that the plot legend includes the filenames so that you know which curve goes with which file. Right-click on the legend to change the plotting style, color, linewidth, etc. The zoom and cursor tools can be used to explore an area and pick off data values.

There are buttons which let you save an image of the graph in `BMP` or `JPG` format or print the graph. To select the printer, select `File→Page Setup→Printer`

`setup` from the menu bar at the top of the screen. This is a LabVIEW function and so may be done from any LabVIEW program.

If, while the program is running, you change one of the files outside the program, hit the Refresh Paths button to re-read the file. This program and 2-Column Editor remember the same default directory, which is not necessarily that used by the EXAFS or XRF programs.

III. Weighted sums

Figure 2 shows the tab for sums and products. In this example, we are taking the difference between the data in the file `cr2o3.b` and that in `cr2o3.f` by adding them with weights 1 and –1 according to Equation 1). If the Mode switch had been in Π position instead of Σ, it would have been a weighted product according to Equation 2). As you can see from this example, the weights are set by the controls down the side of the plot, which correspond to the files in the path indicator.

For a weighted sum, there's no restriction on the data. However, for a weighted product, special care has to be taken for negative or zero operands. If the weights (powers) are non-integer, then negative data would make no sense. However, if the powers are integer, then the data can be negative. Fortunately, the LabVIEW exponentiation operator does the right thing when given an integer power.

As stated above, the data are pruned and interpolated so that the domain of the result (limits of the abscissa) is the intersection of the domains of the inputs. The data are interpolated to the grid of the first file using a cubic spline algorithm with vanishing second derivatives assumed at the ends. It is sometimes useful to resample a file onto the grid of another. You can do this by setting the 'template' file as the first one, but giving it zero weight.

To save the result, push the `Save` button and a file dialog will appear.

IV. Adjusts

The program lets you apply a linear gain and offset to either X or Y for any file, which can be handy for such things as making stack plots and comparing raw EXAFS data files with differing edge jumps and pre-edge backgrounds. The X adjustment is

useful for shifting XANES files to compensate for drifting calibration and for comparing raw EXAFS files done with my convention (energy in eV) and the WinXAS convention (energy in keV). These adjustments are independent. To set the adjustment, click on one of the elliptical Adj? radio buttons just to the right of the checkboxes. This will bring up a set of controls as seen in Figure 3. There are two sets of controls, one for Y and one for X. Since it's more common to adjust Y, the Y adjusts are on top. The adjustments are gain and offset, with the gain applied first (Y*gain+offset, not (Y+offset)*gain). Since gains and offsets might have to take on very large or small values, each is expressed as a fine control times a power of two times a power of 10. Thus, to get an offset of 200, you could set the offset control to 0.2, the offsetx2^n control to 0 and the offsetx10^n control to 3 ($0.2x2^0x10^3$=200), or the offset control to 0.5, the offsetx2^n control to 2 and the offsetx10^n control to 2 ($0.5*2^2*10^2$=200). Note that when you adjust one file, the other files keep their adjustments. Thus, you can make a waterfall plot by adjusting the files in succession.

One often wants finer control than what can be gotten by moving the sliders around. That's where the little green buttons to the left of the gain&offset controls come in. Note that each button has an arrow in it. The left-hand button with the left-pointing arrow expands the range of the corresponding slider to the left (minimum value), and the one with the right-pointing arrow contracts the range on the left. Similar things happen for the buttons on the right. This behavior becomes obvious and intuitive when you play with the buttons and see what happens to the controls. If running the source-code version, which is what's on the Desktop on UXAS_DATA, then you can type in numbers for the min and max values.

The Reset this button resets the gain and offset of the file whose controls are displayed to 1 and 0, respectively. The Reset all button does this to all files.

These adjusts carry over to the Sum&Product screen. Thus, one can use the sliders to do a fine adjustment on the proportion of one file subtracted from another, and see the results as the adjustment is done.

V. Overabsorption

There is a version of this program which implements a simple, adjustable overabsorption correction, modeled on the formula for the effect in a thick, flat sample. This formula may be expressed as

$$y_{OA} = \frac{y}{1 - b + b\,y} \tag{3}$$

where y is the pre-edge subtracted, post-edge normalized signal which would be measured in the absence of overabsorption (OA), y_{OA} is what's measured in the presence of overabsorption, and b is a dimensionless parameter which measures the strength of the effect and depends on the absorption coefficients below the edge, above the edge, and at the fluorescence energy, as well as the takeoff and incidence angles. Now, this equation may be inverted to yield

$$y = \frac{y_{OA}}{1 + a - ya} \tag{4}$$

where

$$a = b\,/\,(1 + b) \quad . \tag{5}$$

In the OA-enabled version of the program, an extra adjustment slider allows you to impose the transformation (4) with adjustable α, thus "undoing" any desired amount of OA, as long as the effect is really describable by the simple model. Now, although real samples have topography and a distribution of takeoff angles, making the simple model invalid in principle, it still works quite well as an empirical correction in practice. Similarly, a mild hole effect may be corrected using this method. Of course, one does not generally know a priori how much correction to use, so the usual procedure is to correct to match references. This same idea, with the same math, is used in the linear fit program.

The adjustment with a positive α 'undoes' OA, and using a negative value, one can simulate the effect.

There are two versions of the program partially for historical reasons, and partially because it's often useful to have two separate plot-add-multiply screens up at the same time and LabVIEW doesn't allow multiple instances of the same program.

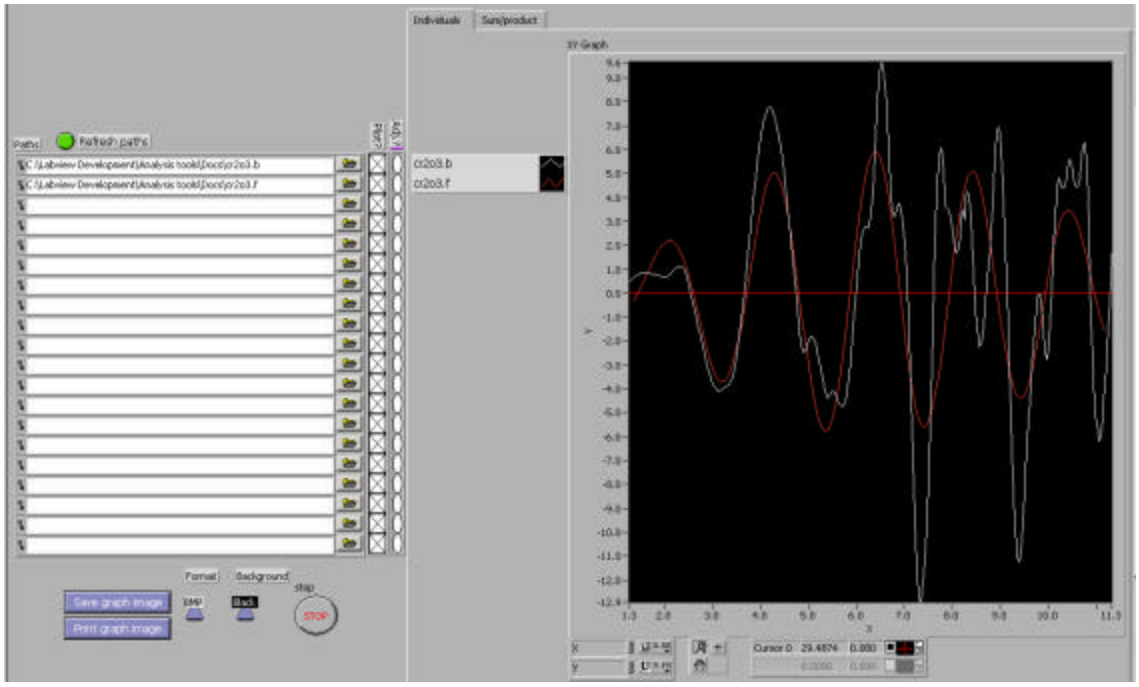

Figure 1. The plot screen with the file controls. The red line is the cursor.

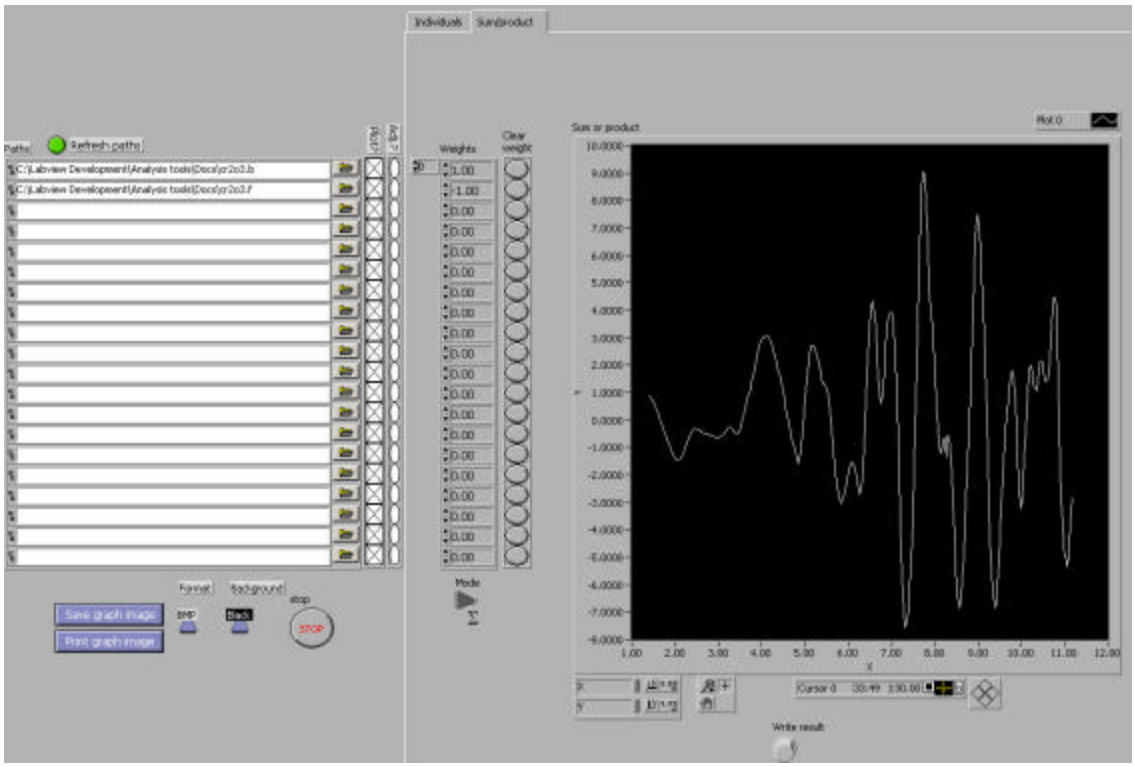

Figure 2. The sum-and-product screen, showing a weighted sum: `1*cr2o3.b+(-1)*cr2o3.f`. *It's a sum because the Mode switch is in the* Σ *position instead of* Π .

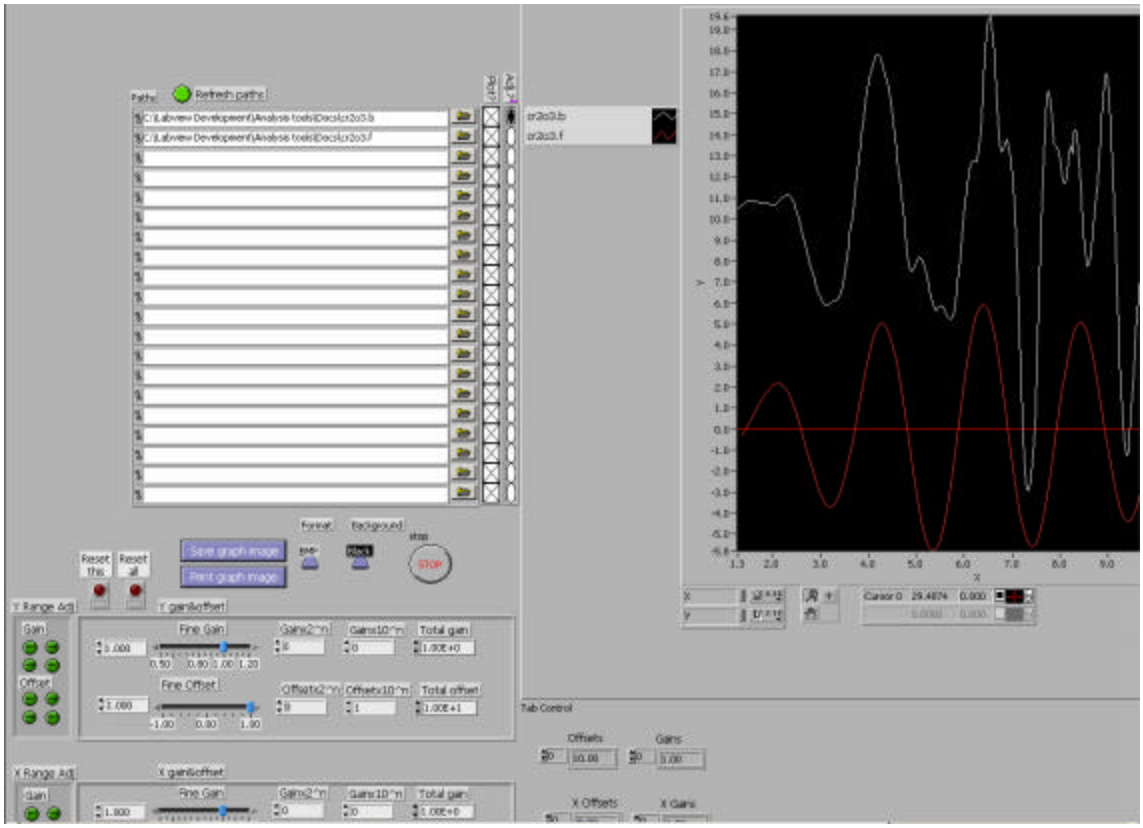

Figure 3. The main screen with the adjusts enabled for the first file (plotted in white). The gain is 1 and the offset is +10.