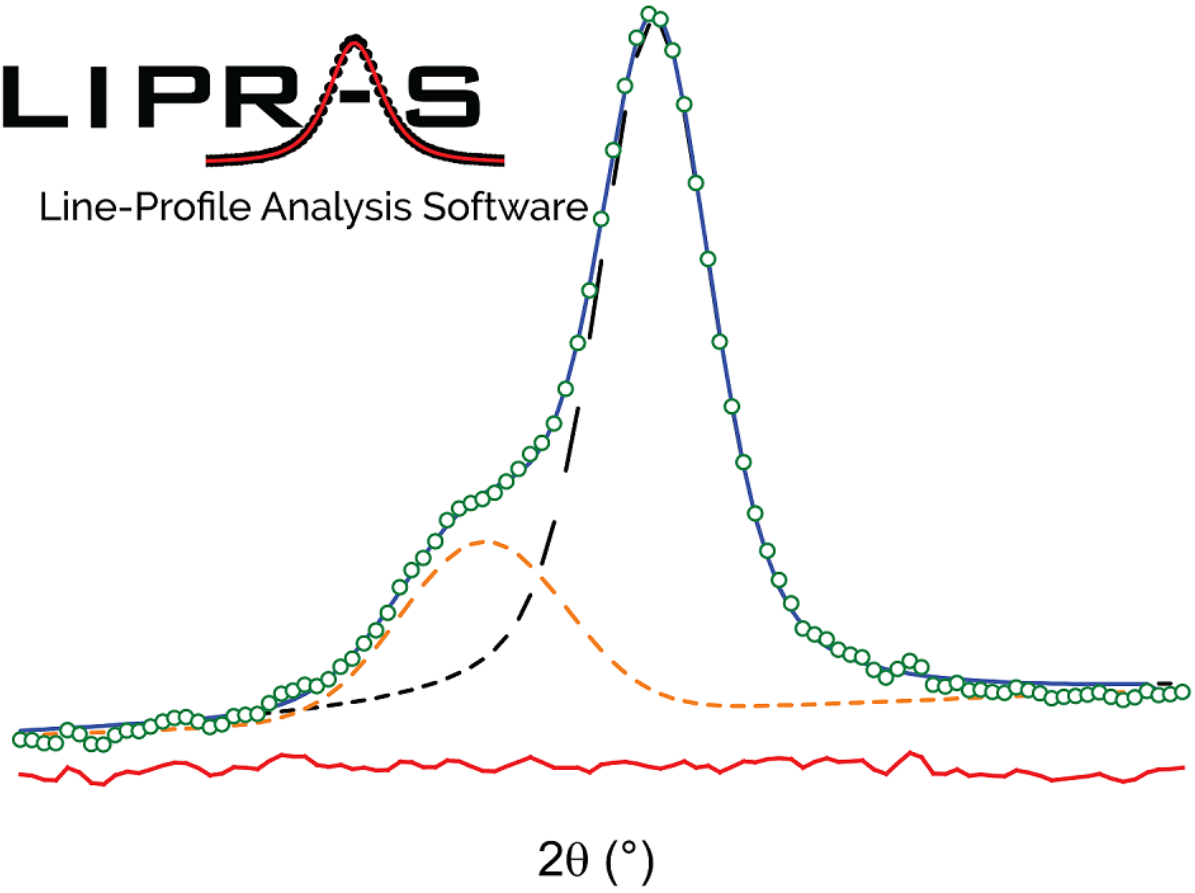
Manual Last Updated: 02-05-2026

LIPRAS
Line-Profile Analysis Software



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I. History

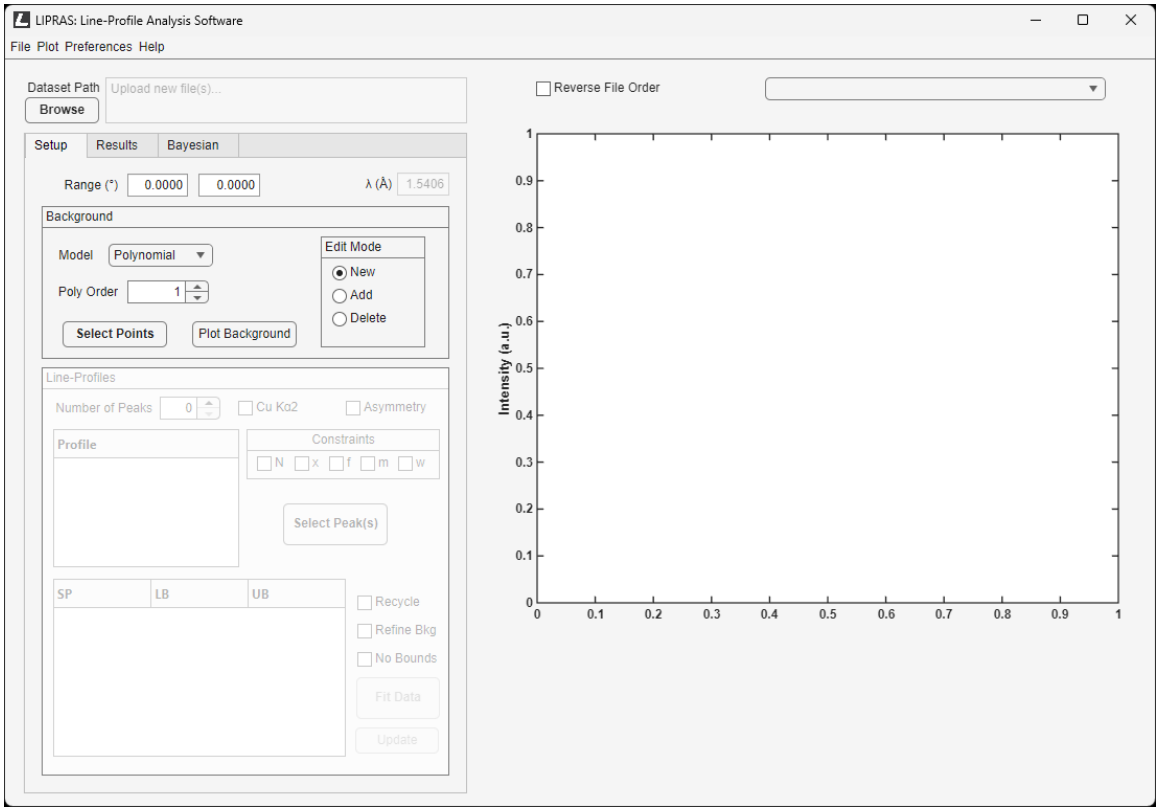
LIPRAS began in 2006 when Jacob Jones, then a postdoctoral researcher, created the core MATLAB code for background subtraction and single peak fitting. In 2014, Chris M. Fancher extended Jacob's work by converting it into a MATLAB class, improving customizability and making new features easier to implement. Giovanni Esteves later refined and expanded this version, adding functionality and polishing the workflow for new users. In 2016, Klarissa Ramos joined the Jones Research Group and, together with Giovanni, refactored the class and developed the first graphical user interface, which became LIPRAS. Today, LIPRAS is solely maintained by Giovanni and has been migrated to MATLAB App Designer.

II. Peak Fitting with LIPRAS

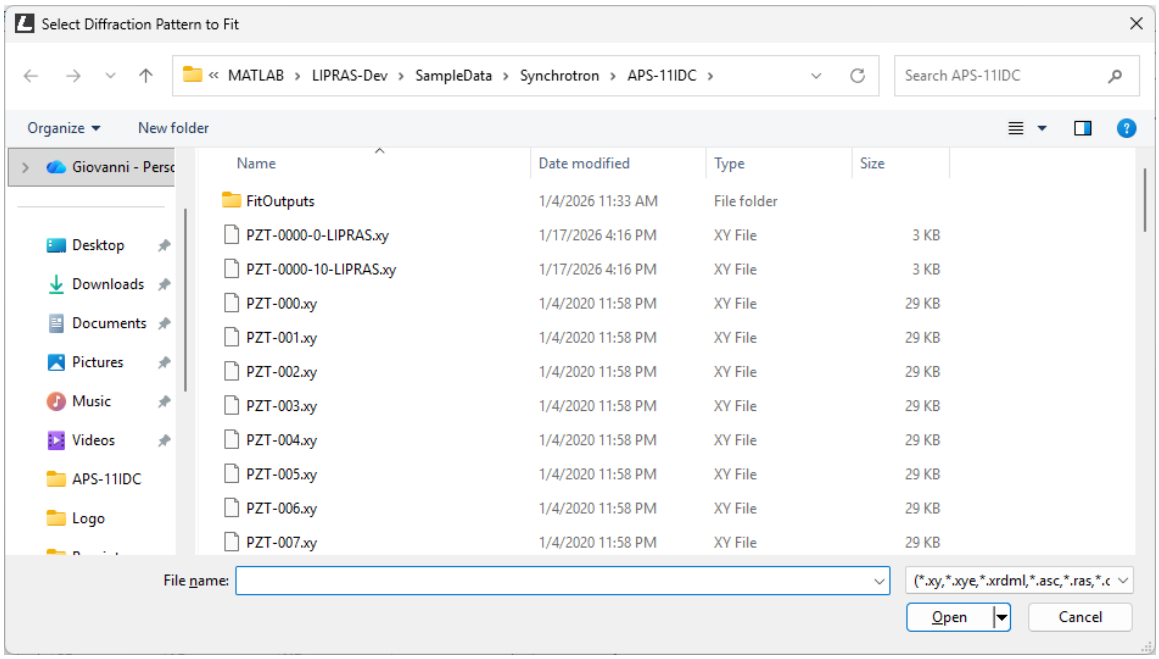
1. Browsing for Data and Accepted Data Files

LIPRAS except data in 2-3 column format. For files of type FXYE, CHI, and XRDML LIPRAS considers these special exceptions since they are generated from known sources that use a consistent file format. The XRDML for example is from Panalytical Laboratory diffractometers, this file type automatically reads in scans and sets the Cu-Kα1 and Kα2 wavelengths automatically upon reading the file. CHI files are from Fit2D which is a well-known program to reduce 2D diffraction images into 1D intensity vs. 2θ diffraction patterns. This file type skips the first 3 lines and begins to read the first 2 columns of data. Lastly, FXYE files come from beamline 11-BM-B of the Advanced Photon Source at Argonne National Laboratory. These files have 3 columns of 2θ, intensity, and error. The file formats XY and XYE cannot have any headers. The XY file type reads in two column data of 2θ and intensity while the XYE reads in 3 columns of 2θ, intensity, and error. The last file types, XLSX, XLS, and CSV (Windows OS only) are Excel files. These can have some header to them but it is recommended that it be limited to 4 lines or less. In any case, the best scenario is if these files do not have any header at all and are just 2 or 3 column formats of X,Y or X,Y,Error.

Click the ‘Browse’ button to begin



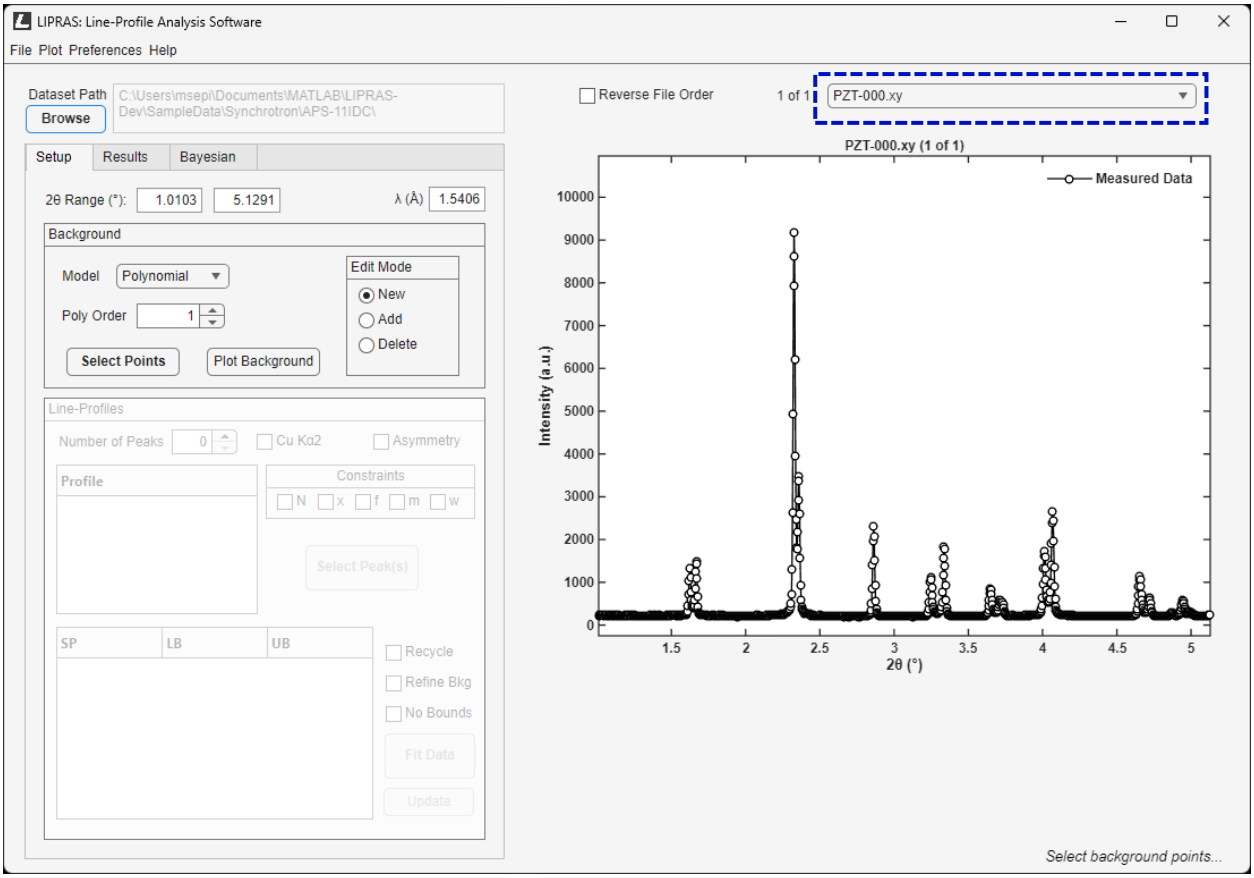
The File Explorer will prompt the user to select the data files



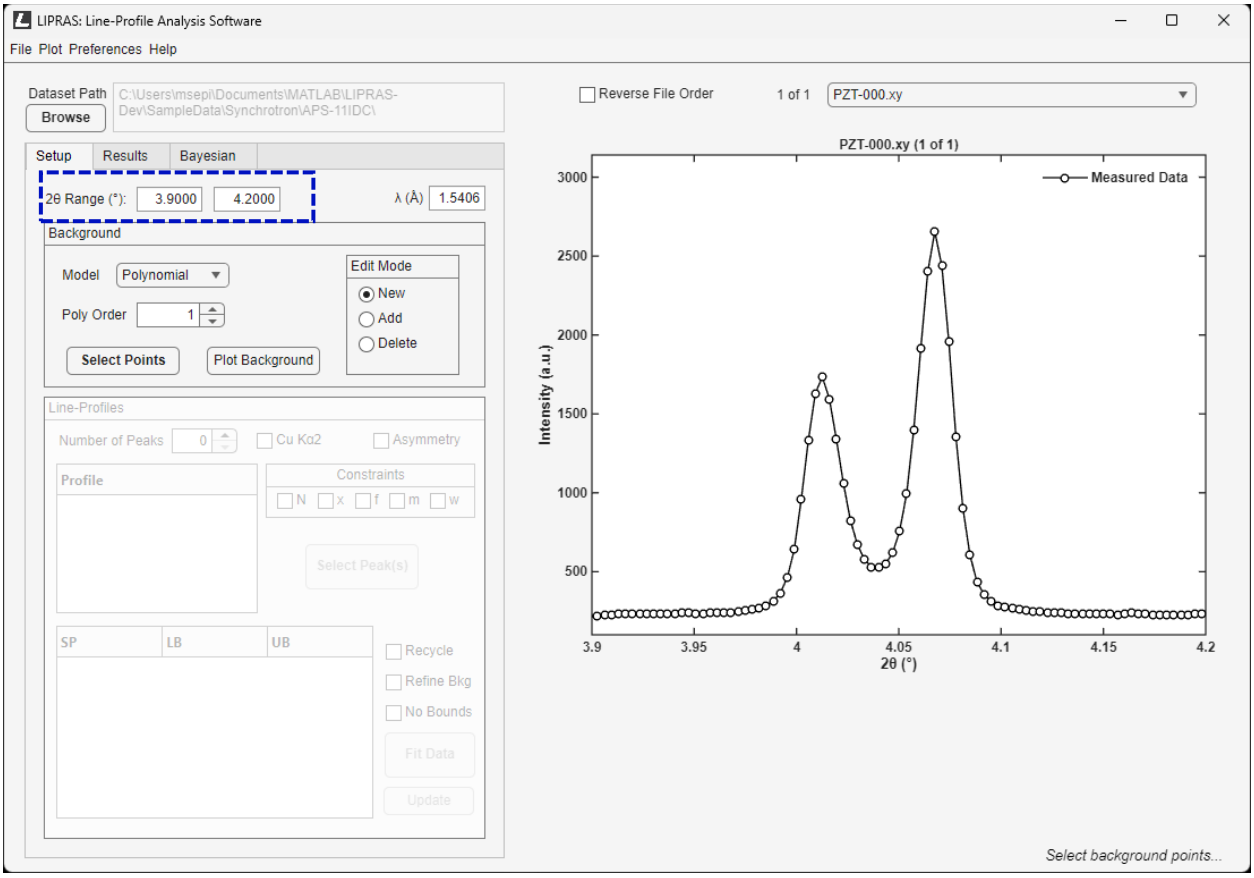
2. Setting the Fit Range and Selecting a Background

After loading a dataset, the plot window will show the first file that was loaded. All files can be viewed by selecting them individually in the drop-down menu, which is boxed in blue on the figure below.

Data loaded can be viewed with the drop down mean (blue box)



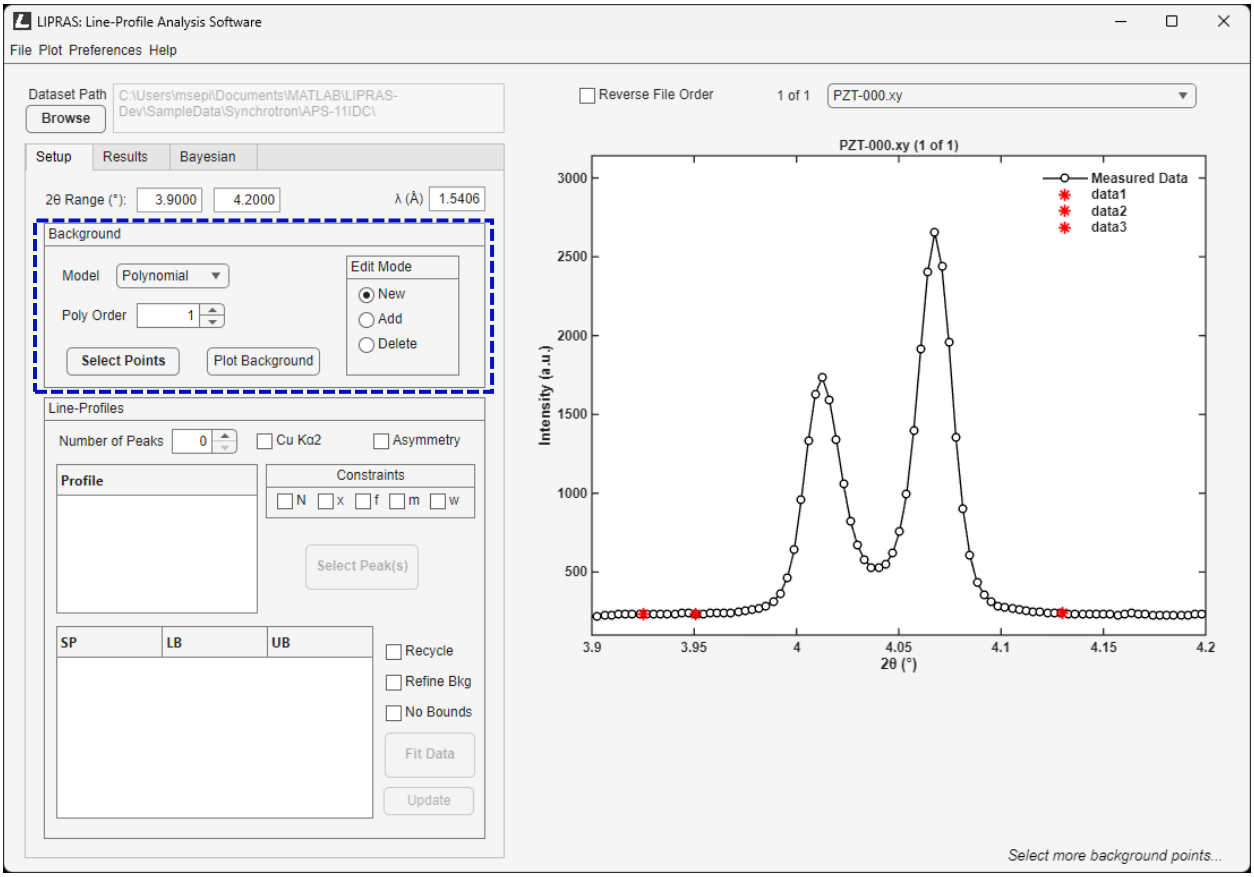
The ‘2θ Range’ can be changed manually, this determines the fit window



Background can be modeled using a polynomial function or a spline function, with background points being user selected. To begin selecting a background, select the ‘Select Points’ button. The cursor will not turn into a crosshair like the previous version. The user may begin selecting points that will be used to model the background only if they are within the figure containing the data. **Note:** The user needs to have more points than the number of polynomial orders. For example, for a polynomial order of 3 at least 4 background points need to be selected. Otherwise, the program will not continue and will prompt the user to select more points. To finish selecting points, press the ‘Enter’ key, and to Cancel and discard all points selected, press the ‘Esc’ key. Points can be added and deleted by toggling the ‘Add’ and ‘Delete’ buttons then clicking ‘Select Points’. Alternatively, the user can right-click at any time to delete a point as well. To view what the background would look like with other polynomial orders, change the polynomial order, and click on ‘Update Plot’. This option helps when dealing with complex backgrounds or when not refining the background

in the least squares routine. The figure below shows a screenshot of the background point selection mode active.

Background points are selected by hitting 'Select Points'



Note: Background point selection is accepted when clicking within the plot. You can click as many points as needed, and when finished 'ENTER' is what stops the process.

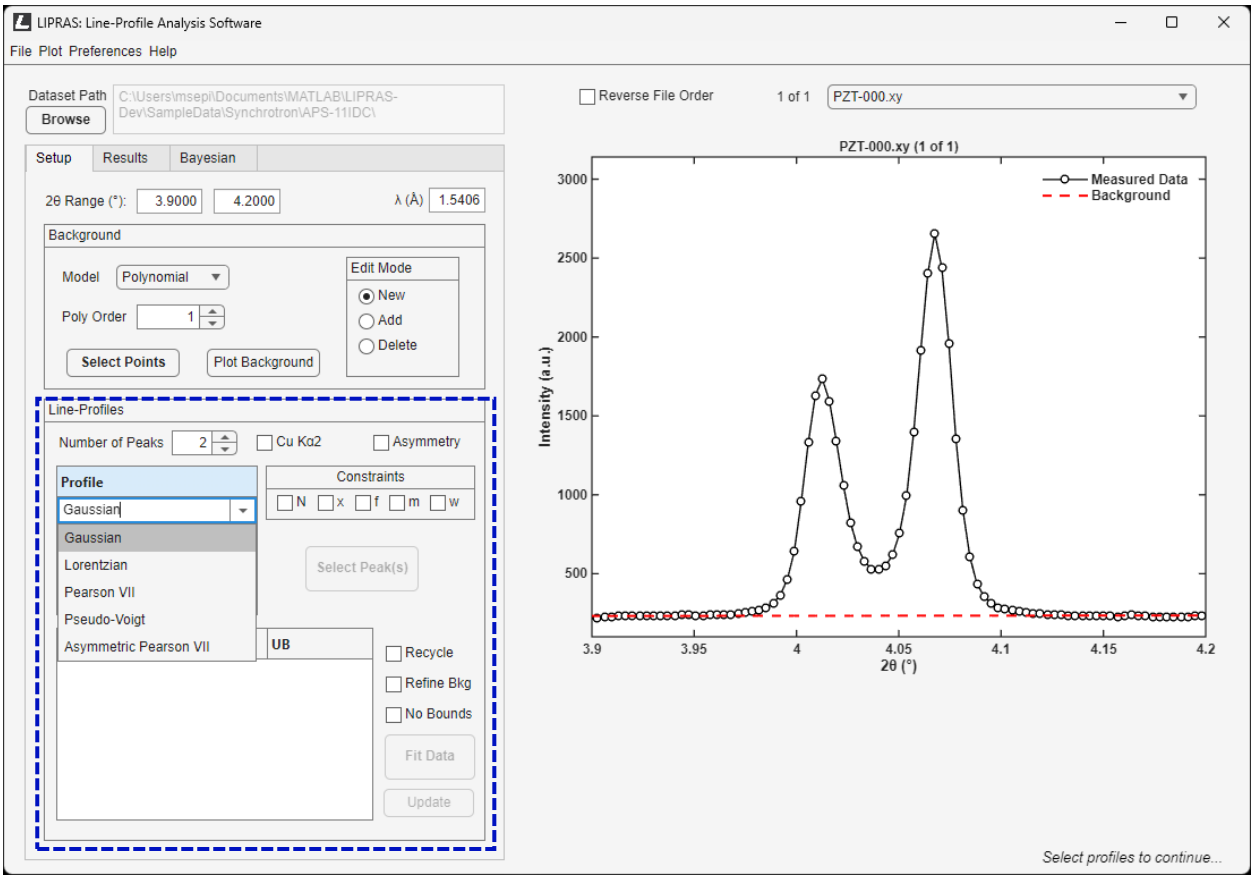
LIPRAS can also include the polynomial background in the least squares routine to refine the background and profile coefficients together. When using the polynomial option, LIPRAS takes advantage of centering and scaling using the average and standard deviation of the 2θ (x) values, see MATLAB's polyfit function for details. Thus, when the background model is refined in the least squares routine the x value is substituted with the Eq. 1 below, where μ_x is the average of all the x values and σ_x the standard deviation.

$$x = \frac{x - \mu_x}{\sigma_x} \qquad 1$$

3. Peaks and Profile Functions

After selecting a background, the number of peaks need to be specified. For each peak introduced in the 'Number of peaks' tab, a profile function needs to be selected. To specify a profile function, click on the empty box that is created upon increasing the number of peaks. This is shown in the figure below.

Selecting Profile functions can be done via a drop-down menu



LIPRAS uses four well-known symmetric line-profile functions and one asymmetric function: Gaussian, Lorentzian, Pearson-VII, pseudo-Voigt, and Split Pearson-VII (asymmetric). The maximum number of peaks that can be applied is 20. Equations 2-5 describe the four symmetric functions in LIPRAS, and are also described in Ref. [1].

Gauss:

$$y(x) = G(x) = \frac{C_G^{1/2}}{\sqrt{\pi}H} \exp\left(-C_G x^2\right) \qquad 2$$

Lorentz:

$$y(x) = L(x) = \frac{C_L^{1/2}}{\pi H}(1 + C_L x^2)^{-1} \quad (3)$$

Pseudo-Voigt:

$$y(x) = PV(x) = \eta G(x) + (1 - \eta)L(x) \quad (4)$$

Pearson-VII:

$$y(x) = PVII(x) = \frac{\Gamma(\beta)}{\Gamma(\beta - 1/2)}\frac{C_P^{1/2}}{\sqrt{\pi}H}(1 + C_P x^2)^{-\beta} \quad (5)$$

- H is the full widths at half maximum (FWHM)

- $x = 2\theta i - 2\theta k/H_k$, Bragg angle of the *i*th point in the diffraction pattern with its origin at the position of *k*th peak divided by the peak's FWHM

- $2\theta_i$ and $2\theta_k$ are the Bragg angle of the *i*th point and the calculated (ideal) Bragg angle of the *k*th Bragg reflection

- C_G=4ln2, C_L=2, and C_p=4($2^{1/\beta}$-1)

- η is the pseudo-Voigt function mixing parameter, where η=1 represents a Gauss function and η=0 a Lorentz function

- Γ is the gamma function

- β exponent that describes the tails of the function, where β=1 is a Lorentz function and with increasing β the function resembles a Gauss function

Each function has its strength and weaknesses in terms of its intrinsic profile. The Gauss function is a symmetrical function and exhibits a Gaussian distribution of the diffraction intensity. The Lorentz function has more pronounced tails compared to the Gauss function. The pseudo-Voigt is a linear combination of the Gauss and Lorentz function and is the most widely used line-profile function used to fit diffraction data. The Pearson-VII function is like a Lorentz distribution, but its profile is altered by the parameter β. Depending on the value of β the profile can be more Lorentzian when closer to 1 and Gaussian when approaching a value of 10.

Peak asymmetry can be encountered in diffraction that is not related to instrumental contribution and is a signal from the sample. In this case, an asymmetric function is needed

to fit the diffraction profile. One option, is a modification of the Pearson-VII function to allow both sides of the function to have different integrated intensities. This is called the asymmetric Pearson-VII which is taken from Ref. [2] and is shown in Eq. 6:

Asymmetric PVII:

$$y(x) = \begin{cases} \frac{N_L}{H_L\sqrt{\pi}}\frac{\Gamma(\beta_L)}{\Gamma(\beta_L - 1/2)}[1 + C_P x^2]^{-\beta_R} & for\ x < x_0 \\ \frac{N_R}{H_R\sqrt{\pi}}\frac{\Gamma(\beta_R)}{\Gamma(\beta_R - 1/2)}[1 + C_P x^2]^{-\beta_R} & for\ x \geq x_o \end{cases} \quad 6$$

where N_L and N_R are the integrated intensities of the left and right-hand side of the line-profile. The following equality must hold true in the case of x=x_0

$$\frac{N_L}{H_L\sqrt{\pi}}\frac{\Gamma(\beta_L)}{\Gamma(\beta_L - 1/2)} = \frac{N_R}{H_R\sqrt{\pi}}\frac{\Gamma(\beta_R)}{\Gamma(\beta_R - 1/2)} \quad 7$$

Rearranging gives one variable as a function of the others:

$$H_R = H_L\frac{N_R}{H_L}\frac{\Gamma(\beta_R)}{\Gamma(\beta_R - 1/2)}\frac{(\beta_L - 1/2)}{\Gamma(\beta_L)} \quad 8$$

The total integrated intensity of the distribution (I_{hkl}) is given as

$$I_{hkl} = \frac{N_L + N_R}{2} \quad 9$$

A modification can be added to all symmetric profile functions, Eq. 2-5, to make them asymmetric. This addition was added to give users more choice when encountering asymmetric peaks that are a result of the sample's contribution to the measured intensity. This option is also very stable when compared to the asymmetric PVII in terms of refining and conducting a Bayesian inference analysis. To make Eqs. 2-5 asymmetric, there is an option underneath the 'Constraints' box, when selecting profile shape functions, called 'Asymmetry' that will enable this option. When this option is checked the FWHM of all reflections that are symmetric are replaced with Eq. 10, which is implemented in Ref. [3]. In Eq. 10, *a* describes the asymmetry of the peak with deviations from 0 leading to larger asymmetry.

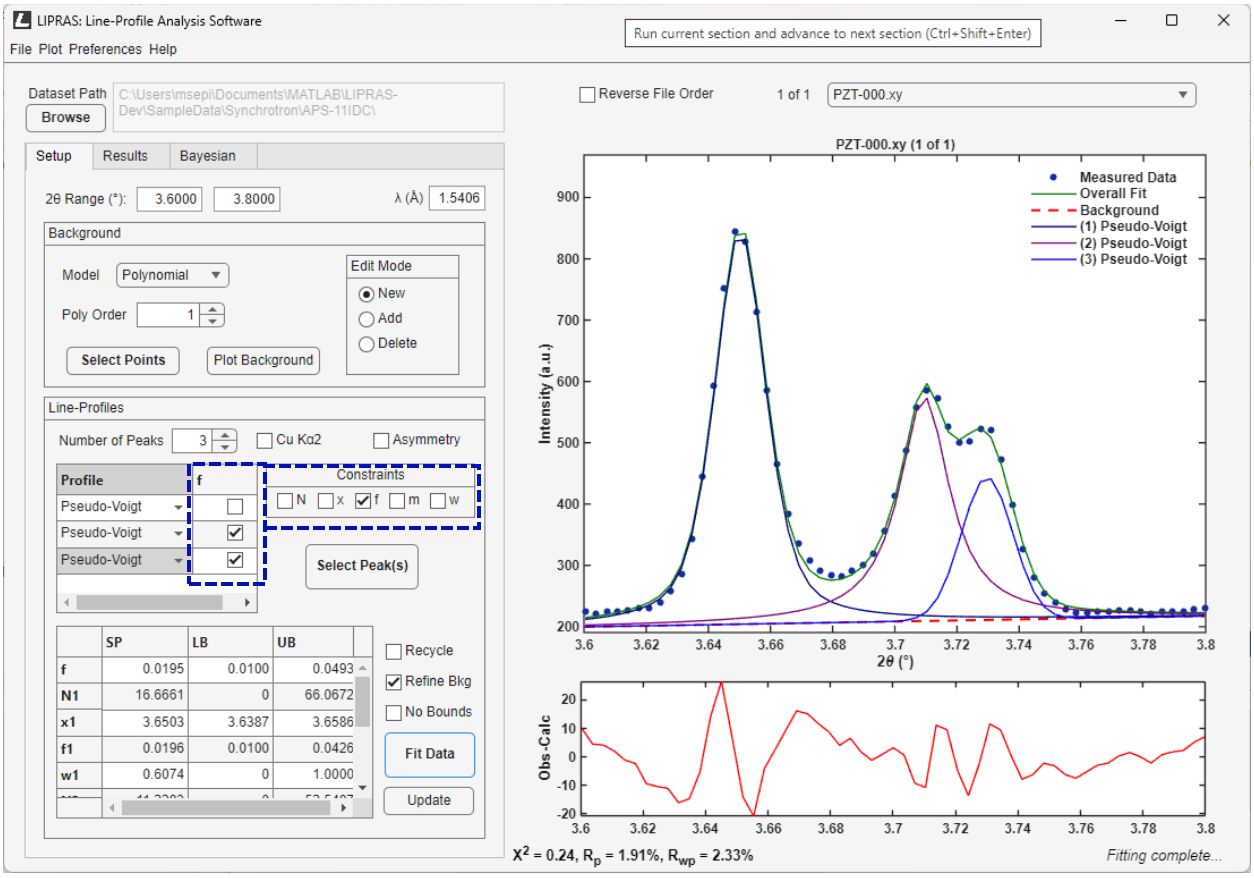
$$FWHM = \frac{2f}{1 + \exp\left(a(2\theta_i - 2\theta_k)\right)} \quad (10)$$

If the data was measured with a laboratory X-ray diffractometer, the respective Cu-Kα2 contributions from each Bragg reflection can be calculated and accounted for in the fit. Files with the extension XRDML automatically activate this feature of LIPRAS and read in the corresponding Cu-Kα1 and Kα2 wavelengths from the file. However, if the files are not XRDML or there is not Kα2 component this feature can be manually activated/deactivated.

i. Constraining Profile Coefficients

One of the strong suits of LIPRAS is its ability to constrain profile coefficients to be equal. For example, an analysis can be conducted in which the FWHM of two profiles are constrained to be equal. This becomes useful when fitting overlapped Bragg reflections or when mixing coefficients of two pseudo-Voigt or Pearson-VII functions reach an upper or lower bound in the least squares routine. To activate the constraints, select the coefficient to constraint in the constraints panel highlighted in the figure below. To constraint profile coefficients at least two functions must be used, and when using more than 2 profile functions a separate column of checkboxes will appear to select which profile functions the user would like to constrain as shown in the figure below.

Constraining profile coefficients can be checked in the ‘Constraints’ box



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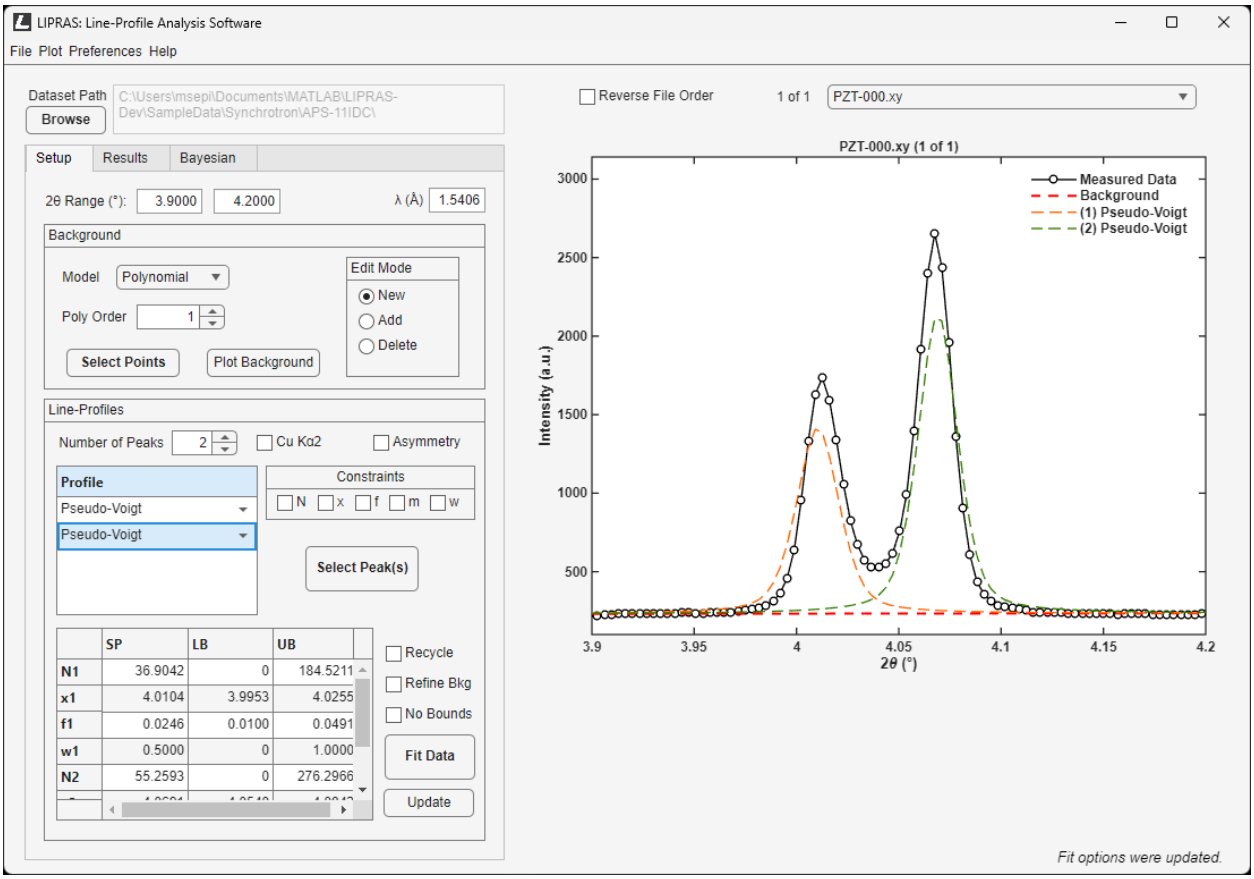
4. Fit Bounds and Options

After peak position(s) have been selected, initial guesses are generated from the peak position(s). The selected profile functions are plotted with the initial guesses in dashed lines. Before starting the fit, starting values for the selected peaks can be adjusted to ensure that the starting parameters are relatively close to the anticipated final solution. After the table in 'Fit Bounds' has been populated, a fit can begin by hitting 'Fit Data'. There are three checkboxes contained within this area of the GUI that allow for more customizable fitting options: Recycle, Refine Bkg, and No Bounds.

After peak position selection initial guess are generated and shown in dashed lines



ii. Recycle

The 'Recycle' feature is very powerful in LIPRAS. When toggled, this feature uses the initial parameters in the table within 'Fit Bounds' and applies them to the first data file. Then,

after a least squares solution is reached for the first file, these results become the starting parameters for the second file. The method repeats until all files have been fitted. This option is recommended when fitting diffraction patterns that have incremental changes with applied stimulus. If this option is not check the values within the 'Fit Bounds' table will be used for every diffraction pattern.

iii. Refine Bkg

Refine Bkg allows the polynomial background model to be included in the least squares routine along with the profile functions selected. The polynomial order is set by the user in the 'Setup' tab. If this option is not checked than the background is determined from the user selected points and subtracted from the raw data before starting the least squares routine. Refining the background with the profile functions typically provides better goodness-of-fit. Therefore, this method is recommended. Typically, this option can be checked with the 'Recycle', but for best results it is suggested to run an initial fit, then hit 'Update' to allow the Starting Parameters to be updated with the results of the previous analysis, then checking 'Refine Bkg' and conducting another fit. More details in the subsequent sections.

No Background in Least Squares: 'Refine Bkg' is <u>NOT</u> Checked,

By considering the intensity, $Y(i)$, of the ith point (where i ranges from 1 to n, n is the total number of measured points) of the diffraction profile, Eq. 11 can be used to model an observed diffraction profile.

$$Y(i) = \sum_{k=1}^{m} I_k[y_k(x_k)] \qquad 11$$

In Eq. 11, I_k is the intensity of kth Bragg reflection, and is dependent on the profile function used to model the pattern y_k whose input is $x_k=2\theta_i-2\theta_k$. The use of a Bragg intensity (I_k) as a multiplier in Eq. 11 allows for analyzing diffraction profiles using normalized functions that are independent of peak intensity. This means that the definite integral of the line-profile function $y_k(x_k)$ integrates to unity, *i.e.* $\int_{-\infty}^{\infty} y_k(x_k)dx = 1$. [1] In this approach, the background is calculated based on the points picked by the user. Once the background is fitted, based on the points, and evaluated, the inputted data is subtracted from the

background and then the model is applied. In this method, the refinement of the background does not take place and this can be used to see clearer trends in the coefficients of the profile function without influence of the background since it's not refined simultaneously with the profile model.

Background in Least Squares: Refine Bkg' IS Checked,

In this method, the background model $b(i)$ is simultaneously refined with the profile model, as shown in Eq. 12. This approach results in better fits than when the background model is excluded from least squares. However, the profile coefficients are dependent on the fit of the background, and in weak signal data or data with complex background, the profile coefficients can fall into false minimum due to the background accounting for the intensity of a peak.

$$Y(i) = b(i) + \sum_{k=1}^{m} I_k[y_k(x_k)]\,; \qquad 12$$

iv. No Bounds

The 'No Bounds' options, when checked, ignore the upper and lower limits specified and only takes the starting parameters as an input. This activates a true Levenberg–Marquardt least squares algorithm to take place instead of the Trust-Region algorithm, which is the default when using upper and lower bound limits. This option should be used with caution when using profile shape functions with mixing coefficients such as pseudo-Voigt and Pearson VII since it can lead to unphysical values or the solution may diverge causing an error. Typically, it is best if the user starts out by refining the profile coefficients first, hitting 'Update', then checking 'Refine Bkg', fitting the data again, hitting 'Update', then select 'No Bounds' while 'Refine Bkg' is checked and hit 'Fit Data'.

5. Fitting Data

To minimize the applied model to the actual data, LIPRAS uses a least squares routine that is part of the Curve Fitting Toolbox™ developed by MathWorks®. This least square fitting method minimizes the difference between the measured diffraction peak and the modeled diffraction profile using least squares minimization. In this method, errors in the parameters

are usually reported as confidence intervals for the estimated parameter values. There are two minimization routines that are used by the Curve Fitting Toolbox™ which depend on whether the coefficients have specified upper and lower bounds or they do not. When the reduction algorithm must abide by the users upper and lower bounds, a Trust-Region-Reflective Least Squares algorithm is used, and when 'No Bounds' is selected the Levenberg-Marquardt Method is used. For more information on these reduction algorithms **click here**.

The reduction algorithm used by LIPRAS allows for the input of weights which means the minimization routine can take errors of the measured intensity into account in the least squares refinement. When errors are properly read in, or when the 'Weights' are defined in the Preference tab as anything but 'None' the least squares algorithm minimize χ^2 since $w=1/\sigma_i^2$ and σ_i is usually the square root of the observed intensity of the ith point.

$$\chi^2 = \sum \frac{(y_{obs} - y_{calc})^2}{{\sigma_i}^2} = \sum w(y_{obs} - y_{calc})^2 \qquad 13$$

To evaluate goodness-of-fit, by default the Curve Fitting Toolbox™ use the following: R-square, adjusted R-square, and root mean squared error. Additionally, LIPRAS also uses statistical metrics that are commonly found in some Rietveld programs such as: R_p, R_{wp}, and reduced chi-square, which are described in the below.

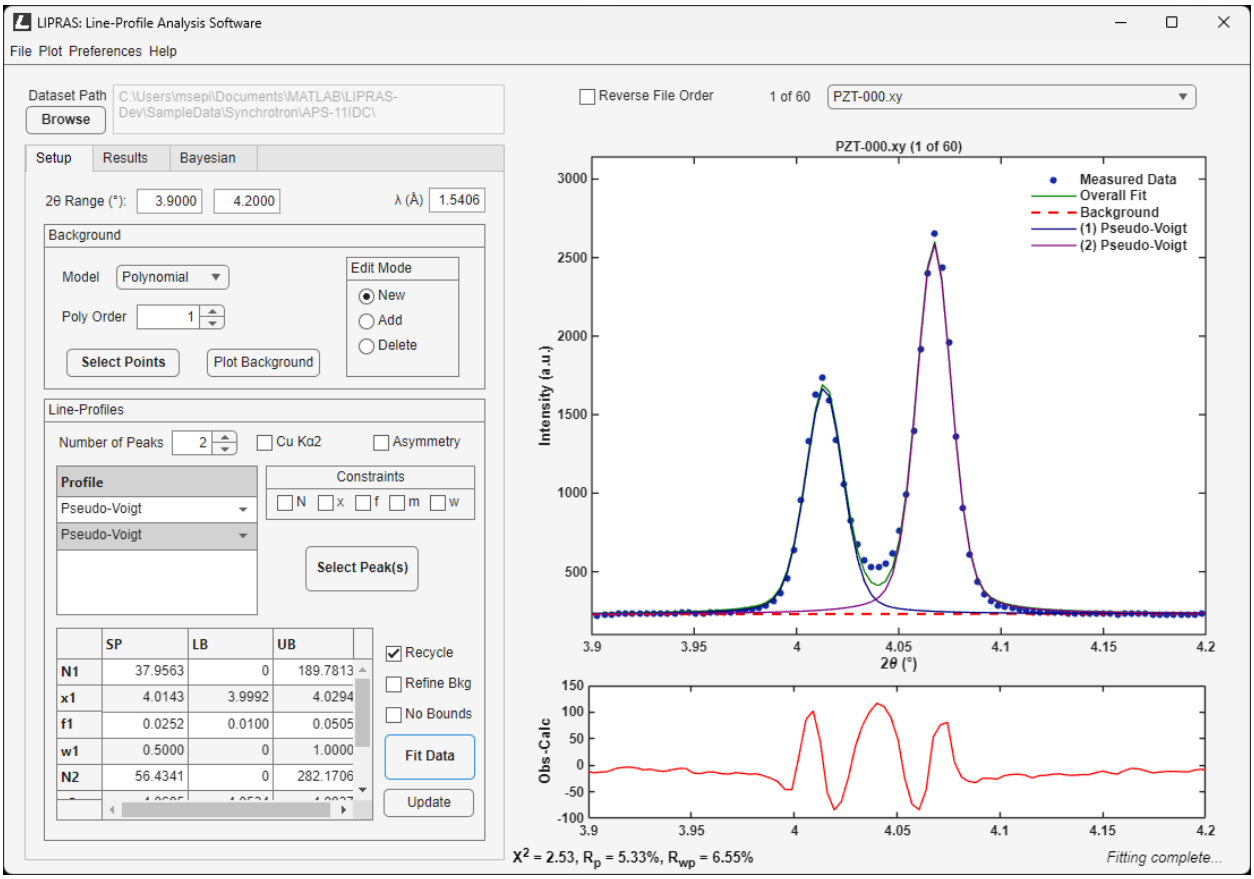
$$R_p = \left(\frac{\sum|y_{obs} - y_{calc}|}{\sum y_{obs}}\right) \times 100 \qquad 14$$

$$R_{wp} = \left[\frac{\sum w(y_{obs} - y_{calc})^2}{\sum w(y_{obs})^2}\right]^{1/2} \times 100 \qquad 15$$

$$\chi^2_{red} = \frac{\chi^2}{v} = \text{GOF} \qquad 16$$

$$v = \#\ of\ data\ points - \#\ of\ variables$$

The resulting fit will automatically display in the GUI window after a fit has finished



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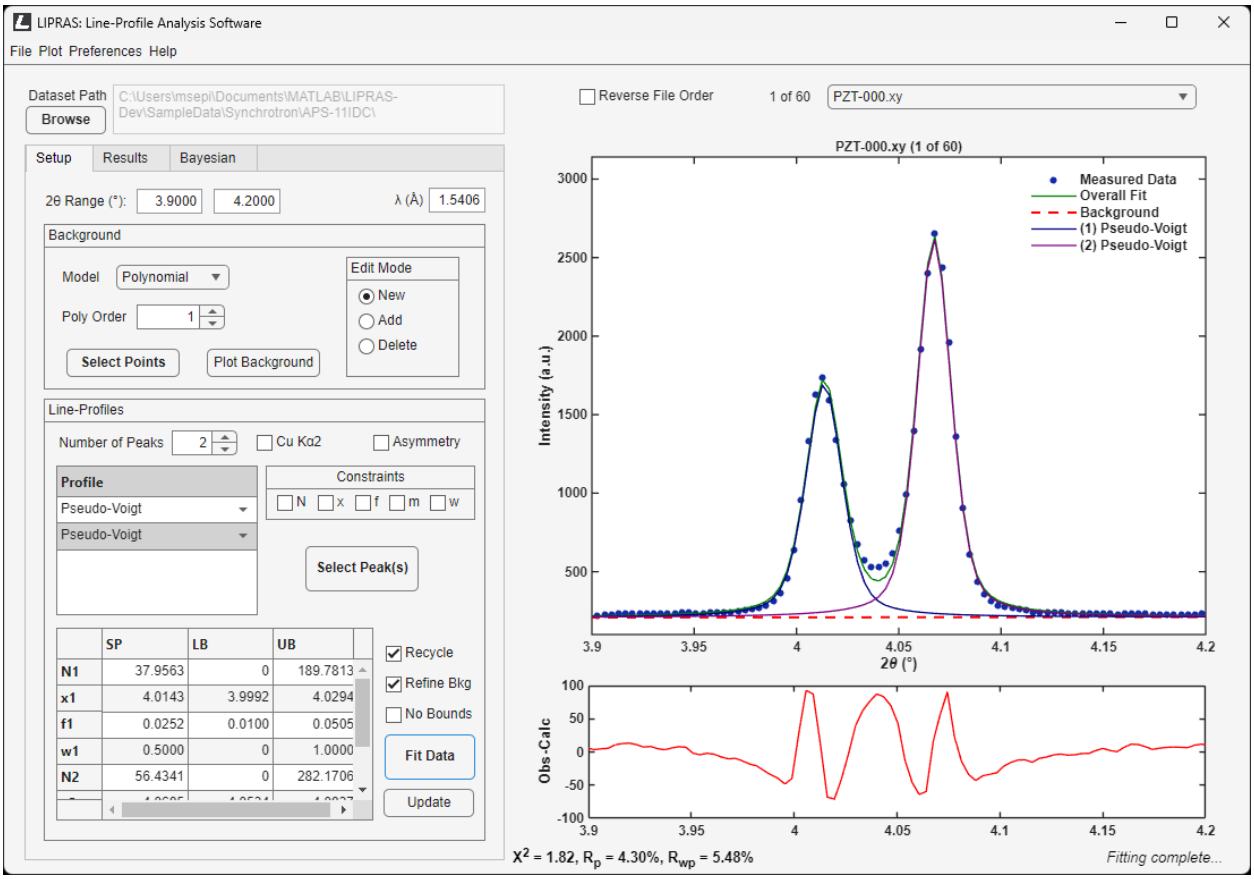
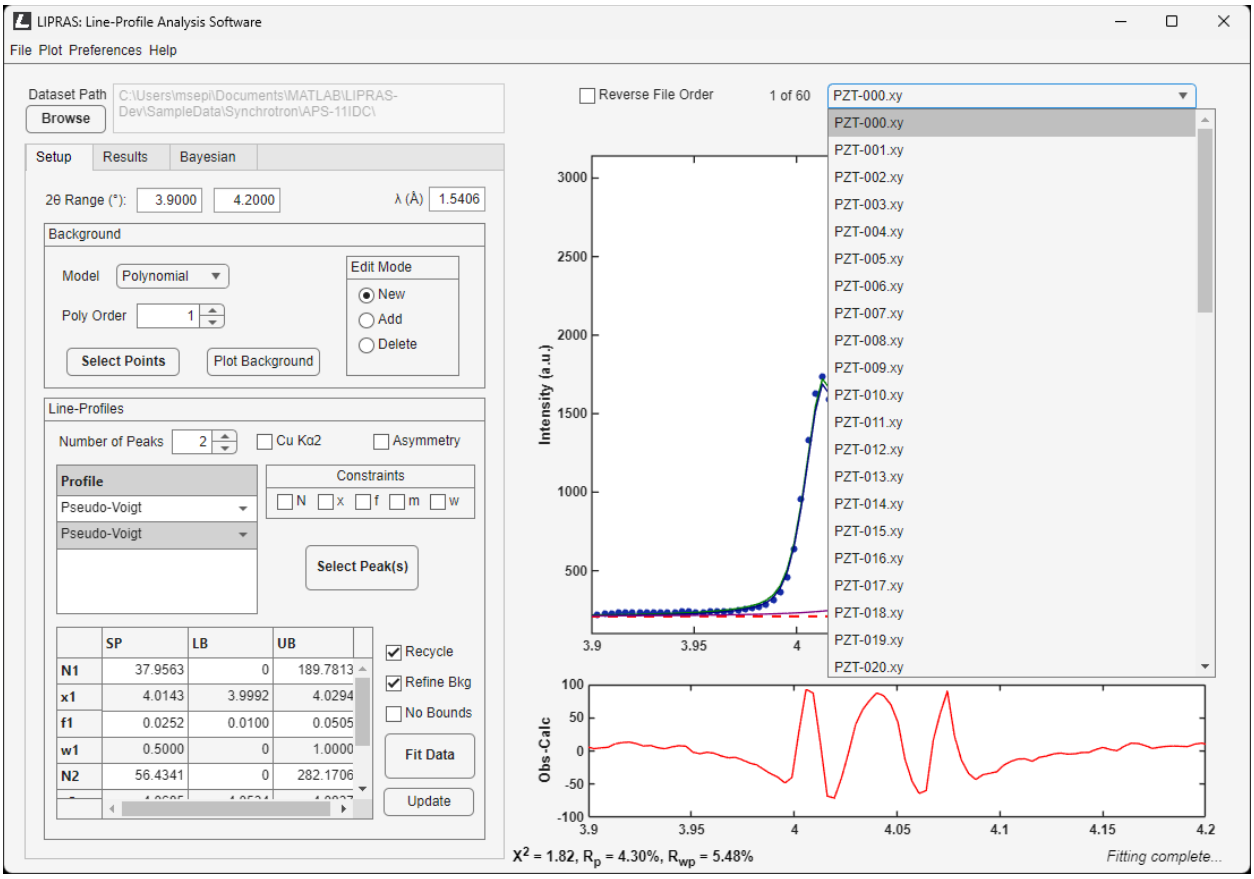
Fit conducted with the background included in the least squares routine



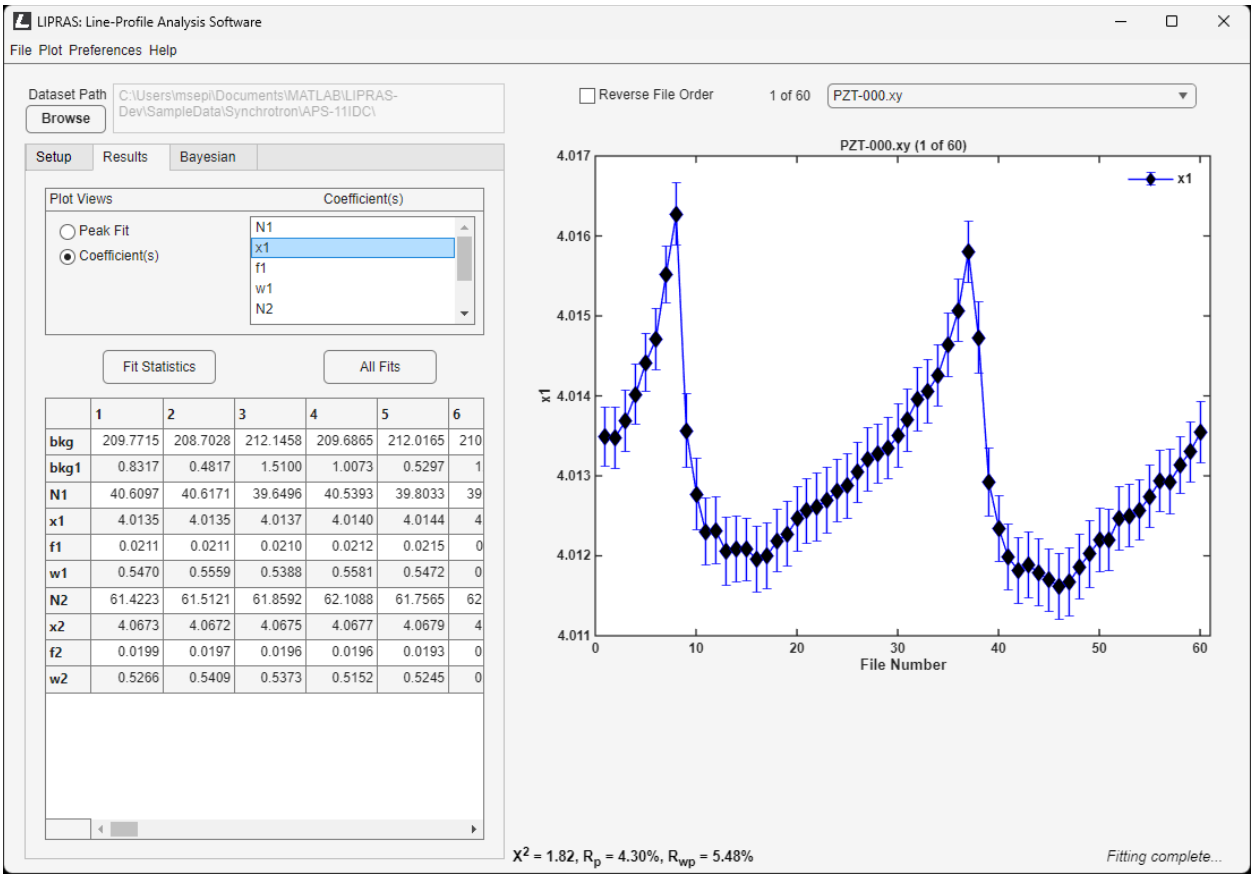
6. Viewing Results

After a fit, the 'Results' tab will become available, which allows the user to view the resulting fit and coefficients as a function of file number. This allows the user to quickly judge the fit and adjust their model or starting parameters. The 'All Fits' button will plot all the fits in one window, but this option should be used with low file numbers, *i.e.* less than 20 files. Lastly, the 'Fit Statistics' button plots the goodness-of-fit statistics as a function of file number, this includes: R-squared, adjusted R-squared, root mean squared error, R_p, R_{wp}, and χ^2_{red}.

View other fits by selecting them in the drop-down or clicking the Results tab



Coefficients vs. file number can be viewed in ‘Coefficient Trends’ in the ‘Results’ tab



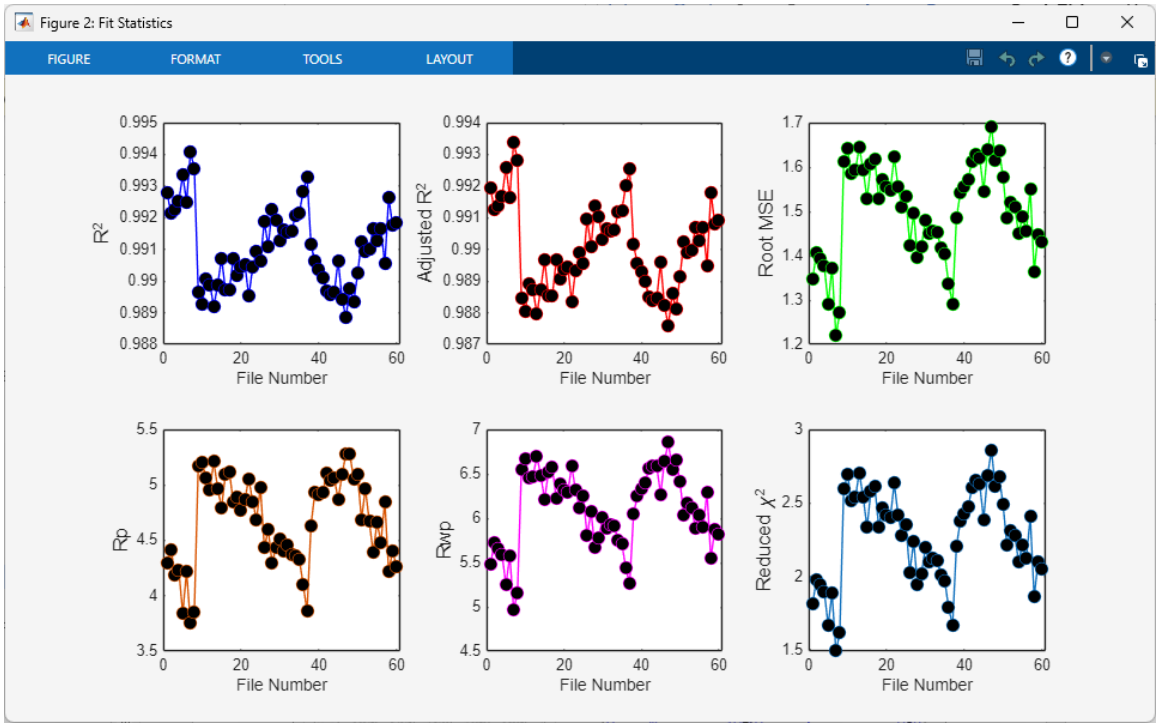
	1	2	3	4	5	6
bkg	209.7715	208.7028	212.1458	209.6865	212.0165	210
bkg1	0.8317	0.4817	1.5100	1.0073	0.5297	1
N1	40.6097	40.6171	39.6496	40.5393	39.8033	39
x1	4.0135	4.0135	4.0137	4.0140	4.0144	4
f1	0.0211	0.0211	0.0210	0.0212	0.0215	0
w1	0.5470	0.5559	0.5388	0.5581	0.5472	0
N2	61.4223	61.5121	61.8592	62.1088	61.7565	62
x2	4.0673	4.0672	4.0675	4.0677	4.0679	4
f2	0.0199	0.0197	0.0196	0.0196	0.0193	0
w2	0.5266	0.5409	0.5373	0.5152	0.5245	0

7. Fit Statistics

The ‘Fit Statistics’ button summarizes how fit quality varies across the dataset by plotting key metrics versus file number. Since this is primarily a peak fitting tool for diffraction data, Rp and Rwp are the primary fit statistics to watch: both are widely used in diffraction, and Rwp is especially meaningful because it includes the same weighting used in the least weighted squares refinement. R^2 and adjusted R^2 provide a complementary measure of how well the model explains the measured profile (with adjusted R^2 accounting for model complexity), while RMSE reports the typical residual magnitude in the data’s units. Reduced χ^2 indicates goodness of fit relative to the assumed uncertainties, with values near 1 suggesting the error model is reasonable. For a more complete description of errors, use the Bayesian feature, which reports out a mean and sigma for each coefficient.

While Rp, Rwp, and the other fit statistics should generally be minimized, the main goal of peak fitting is for the profile function to accurately represent the measured data. At a minimum, the fit should reliably capture the features you care most about, such as intensity, peak position, and FWHM. Peak tails are often overlooked in practice, especially for low signal to noise data, even though they can meaningfully affect extracted widths, background, and integrated intensity.

Fit Statistics for all fits



8. Exporting Results: Fmodel and Fdata Files

Once a fit has been completed, the resulting profile coefficients and data are saved in the directory where the raw data is located. To view the resulting profile coefficients outside of LIPRAS, there is an Fmodel file containing the resulting profile coefficients for all files that were fit in the analysis. An example of an Fmodel file is shown in the figure below. Each Fmodel file will contain the resulting profile coefficients and error. The error is calculated using the 95% confidence interval and subtracting it from the resulting value. Other useful goodness-of-fit statistics are also printed in this file such as R-squared, Adjusted R-squared,

root mean squared error, R_p, R_{wp}, and reduced χ^2 (χ^2_{red}). To open this file, it is recommended to use a text editor. The authors recommend **Notepad++** for Windows users.

Example of an Fmodel File

```
This is an output file from a MATLAB routine.
The following peaks are all of the type: Pseudo-Voigt; Pseudo-Voigt;

FileName    N1  N1_Error    x1  x1_Error    f1  f1_Error    w1  w1_Error    N2  N2_Error
PZT-000_xy  23.34989    1.24188 1.62403 0.00022 0.01619 0.00070 0.53461 0.14240 23.51645
PZT-001_xy  23.19547    1.23743 1.62385 0.00022 0.01594 0.00072 0.56641 0.14226 24.30896
PZT-002_xy  21.68311    1.23785 1.62402 0.00023 0.01630 0.00070 0.44673 0.15627 23.49282
PZT-003_xy  21.01769    1.05110 1.62380 0.00019 0.01617 0.00060 0.41716 0.13806 24.40783
PZT-004_xy  21.99913    1.24187 1.62393 0.00023 0.01640 0.00074 0.52092 0.15114 24.37067
PZT-005_xy  20.73420    1.08835 1.62398 0.00021 0.01642 0.00067 0.47747 0.14238 24.07851
PZT-006_xy  20.03252    1.15473 1.62402 0.00024 0.01645 0.00079 0.56391 0.15276 24.79723
PZT-007_xy  20.17317    1.41575 1.62416 0.00031 0.01760 0.00100 0.55137 0.18524 26.92044
PZT-008_xy  25.94919    1.58788 1.62485 0.00025 0.01712 0.00077 0.46877 0.16364 22.59879
PZT-009_xy  28.01257    1.54085 1.62485 0.00022 0.01635 0.00068 0.49842 0.14474 21.25452
PZT-010_xy  27.79291    1.51445 1.62464 0.00021 0.01584 0.00066 0.49180 0.14510 20.95588
PZT-011_xy  29.11020    1.50519 1.62455 0.00020 0.01560 0.00064 0.52923 0.13717 21.47010
```

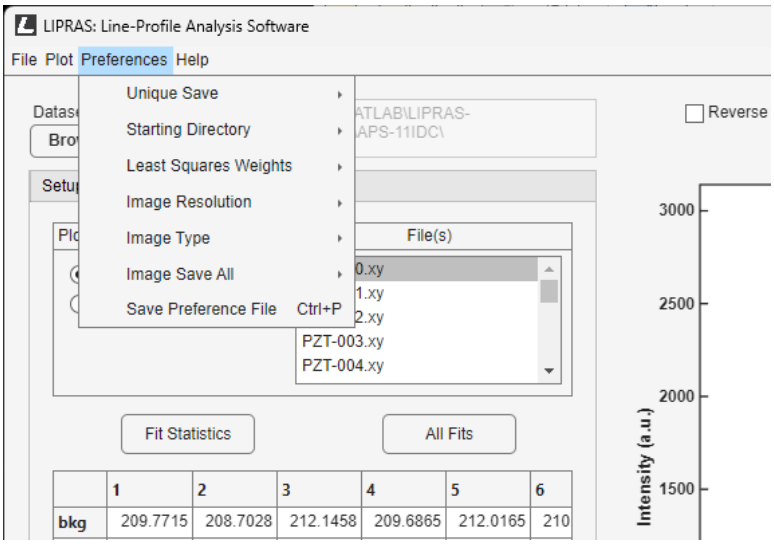
The Fdata file contains the raw data and the evaluated profile function with individual peaks. An example of an Fdata file is shown in the figure below. The columns that are printed with all Fdata files are 2θ, Obs, Calc, BkgdFit, PredIntLow, PredIntHigh, Weights, and Peaks. The PredIntLow and PredIntHigh are the upper and lower 95% prediction bounds for response values from the least squares results. This is done by using the predint function in MATLAB. The peaks column are the evaluated profile functions with the resulting coefficients. The sole purpose of the Fdata file is to create high quality figures of the resulting fits for posters, presentations, and publications.

Example of a Fdata File

```
This is an output file from a MATLAB routine.
All single peak data (column 3+) does not include background intensity.

2Theta    Obs      Calc     BkgdFit     PredIntLow      PredIntHigh     Weights     Peak1    Peak2
1.50156700  229.84500000    2.66234755  221.48915779    0.44935355  4.87534154  0.00435076  1.90748390  0.75486364
1.50500300  229.68100000    2.80570969  222.02561674    0.58498727  5.02643212  0.00435386  2.01858021  0.78712948
1.50843800  221.45000000    2.96111578  222.55922102    0.73149833  5.19073322  0.00451569  2.13961857  0.82149720
1.51187300  220.37900000    3.13002254  223.08965074    0.89012506  5.36992001  0.00453764  2.27185847  0.85816406
1.51530800  222.81400000    3.31406281  223.61642954    1.06223671  5.56588891  0.00448805  2.41672318  0.89733963
1.51874300  224.39100000    3.51512681  224.13908108    1.24940086  5.78085275  0.00445651  2.57586893  0.93925788
1.52217800  229.19100000    3.73541277  224.65712899    1.45341892  6.01740663  0.00436317  2.75123208  0.98418069
1.52561300  228.66700000    3.97748981  225.17009691    1.67636958  6.27861003  0.00437317  2.94508786  1.03240194
1.52904800  218.24100000    4.24437616  225.67750850    1.92066208  6.56809025  0.00458209  3.16012387  1.08425230
1.53248400  209.70800000    4.53972821  226.17903242    2.18918430  6.89027212  0.00476854  3.39960647  1.14012174
1.53591900  222.47000000    4.86761339  226.67390029    2.48506612  7.25016066  0.00449499  3.66721325  1.20040014
1.53935400  230.96500000    5.23318353  227.16178260    2.81225157  7.65411548  0.00432966  3.96760097  1.26558256
1.54278900  231.80900000    5.64254595  227.64220301    3.17532824  8.10976367  0.00431390  4.30633088  1.33621507
1.54622400  231.13000000    6.10311261  228.11468515    3.57977566  8.62644956  0.00432657  4.69019080  1.41292181
1.54965900  223.97100000    6.62395183  228.57875267    4.03219413  9.21570952  0.00446486  5.12753308  1.49641874
```

9. Preferences Menu



Toggle Unique Save: Creates a new folder every time 'Fit Data' is hit

Set Starting Directory: Set the starting directory when browsing for data

Least Squares Weights: Weights involved in least squares routine, as shown **here**. The 'Default' option uses the errors from files that have them. Otherwise, the Weight defaults to '1/obs' if the file does not have errors included.

Image Resolution: Sets the DPI for images that are exported.

Image Type: Sets the image type for exported images

Image Save All: Saves all fits that were conducted, by default LIPRAS will only save the first figure unless this is checked.

10. Input/Output Parameter File

LIPRAS has the option to write an output parameter file that contains the necessary information to recreate the resulting fit. This file can be generated by going to File>Export> Save Fit Parameter file or by hitting CTR+S. This very same file can be imported into LIPRAS after loading data in to recreate and re-populate what was done previously. All output parameter files are of .txt extension and contain the relevant fit information to recreate a fit.

Example of an Output Parameter File

```
2ThetaRange: 11.50000 11.85000

BackgroundModel: Polynomial
PolynomialOrder: 2
BackgroundPoints: 11.502260 11.510655 11.513884 11.518404 11.796079 11.810932 11.820618 11.832242 11.840637 11.846448
Cu-KAlpha1: n/a

Cu-KAlpha2: n/a

FitFunction(s):
Pearson VII; Pearson VII; Pearson VII;
Constraints: {'m'} {'m'} {'m'}
PeakPosition(s): 11.621303 11.647181 11.667884

== Initial Fit Parameters ==
m N1 x1 f1 N2 x2 f2 N3 x3 f3
SP: 1.50000 93.34307 11.62130 0.03045 80.00000 11.64718 0.04169 154.83736 11.66788 0.04047
LB: 0.50000 0.00000 11.60380 0.01000 0.00000 11.62968 0.01000 0.00000 11.65038 0.01000
UB: 20.00000 466.71537 11.63880 0.06090 797.53797 11.66468 0.08339 774.18679 11.68538 0.08094

== Bkg Coeffs ==
SP: -42.48338 -35.96757 183.37026
```

III. Bayesian Inference

A Bayesian inference analysis can be carried out on the resulting least squares results to generate a full description of the errors for all profile parameters. Works best on symmetrical functions, asymmetric function can be a hit or miss. The algorithm used is a Markov Chain Monte Carlo (MCMC) Metropolis-in-Gibbs, which is described in the following paper: **Bayesian** and is now included in every LIPRAS download.

v. Description of Model

Scattered intensity (*I*) is typically measured as a function of scattering angle (2θ), resulting in Bragg peaks

$$I = f(2\theta|\alpha) \quad (1)$$

f is a profile shape function and α is a set of parameters for the profile shape function, which in this case is a pseudo-Voigt, but can be any of the functions listed in **Peaks and Profile Functions**.

$$f(2\theta|\alpha) = \frac{wI\sqrt{4ln2}}{\sqrt{\pi}F} exp\left(-\frac{(4ln2)(2\theta-2\theta_0)^2}{F^2}\right) + 2\frac{I(1-w)}{\pi F}\left(1+\frac{4(2\theta-2\theta_0)^2}{F^2}\right)^{-1} \quad (2)$$

New parameters are generated by $N(\alpha_{st}, s^2)$ which is the normal distribution with mean α_{st} and standard deviation *s*.

$$\alpha_{new} = N(\alpha_{st}, s^2) \quad (3)$$

Bayes Theorem

$$P(\alpha|data) = \frac{P(data|\alpha)P(\alpha)}{P(data)} \quad (4)$$

α is the parameter of interest

P(α|data) is the posterior distribution (probability of parameter values given the data)

P(data|α) is the likelihood (probability of data given the parameter values)

P(α) is the prior distribution

P(data) is the marginal likelihood

$I_{obs,\,j}$ and $I_{cal,\,j}$ is the calculated intensity, *n* is the number of data points and σ^2 is the variance

$$P(data|\alpha) = (2\pi\sigma^2)^{-n/2}\exp\left(-\frac{1}{2\sigma^2}\sum_{j=1}^{n}(I_{obs,j} - I_{cal,j})^2\right) \quad 5$$

Algorithm in LIPRAS:

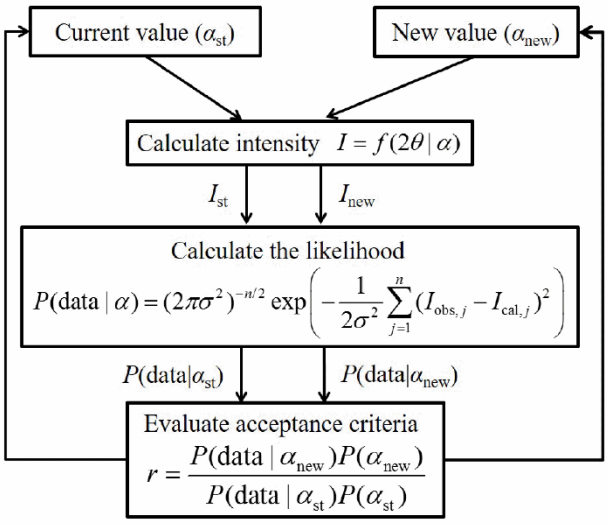


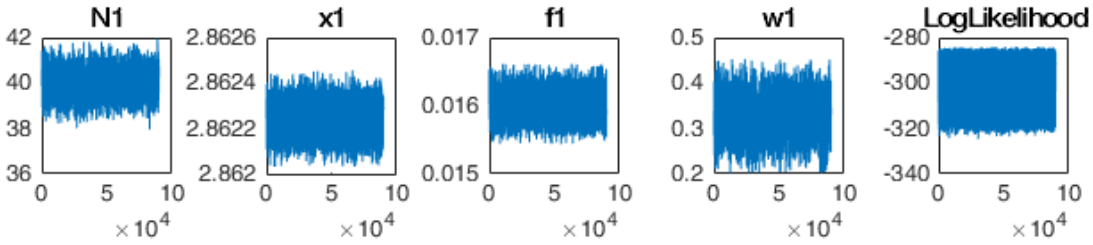
Figure 1 from the following publication: **Bayesian**

vi. Using Bayesian

- Tab to the 'Bayesian' tab after doing least squares fit.
- Table should be populated from results of least squares refinement; you can change these defaults by switching to 'Custom Bounds'. To reset any changes, double-click the 'Default Bounds'.
    - Note: Peak fitting of multiple files will do Bayesian inference on each file. The default parameters are taken individually from each least squares result of each file. If you use 'Custom Bounds' you will apply these bounds to **ALL** files. 'Custom Bounds' is best used for a single file.
    - *Upper and lower bounds* are computed around the parameter mean by applying a scaled standard deviation. The scaling is controlled by the Bounds Multiplier and SD Divider, which widen or tighten the bounds.
    - *Standard deviation (σ)* is initialized from the least squares 95% confidence interval, then globally adjusted using the SD Divider to increase or decrease σ across the entire parameter table.

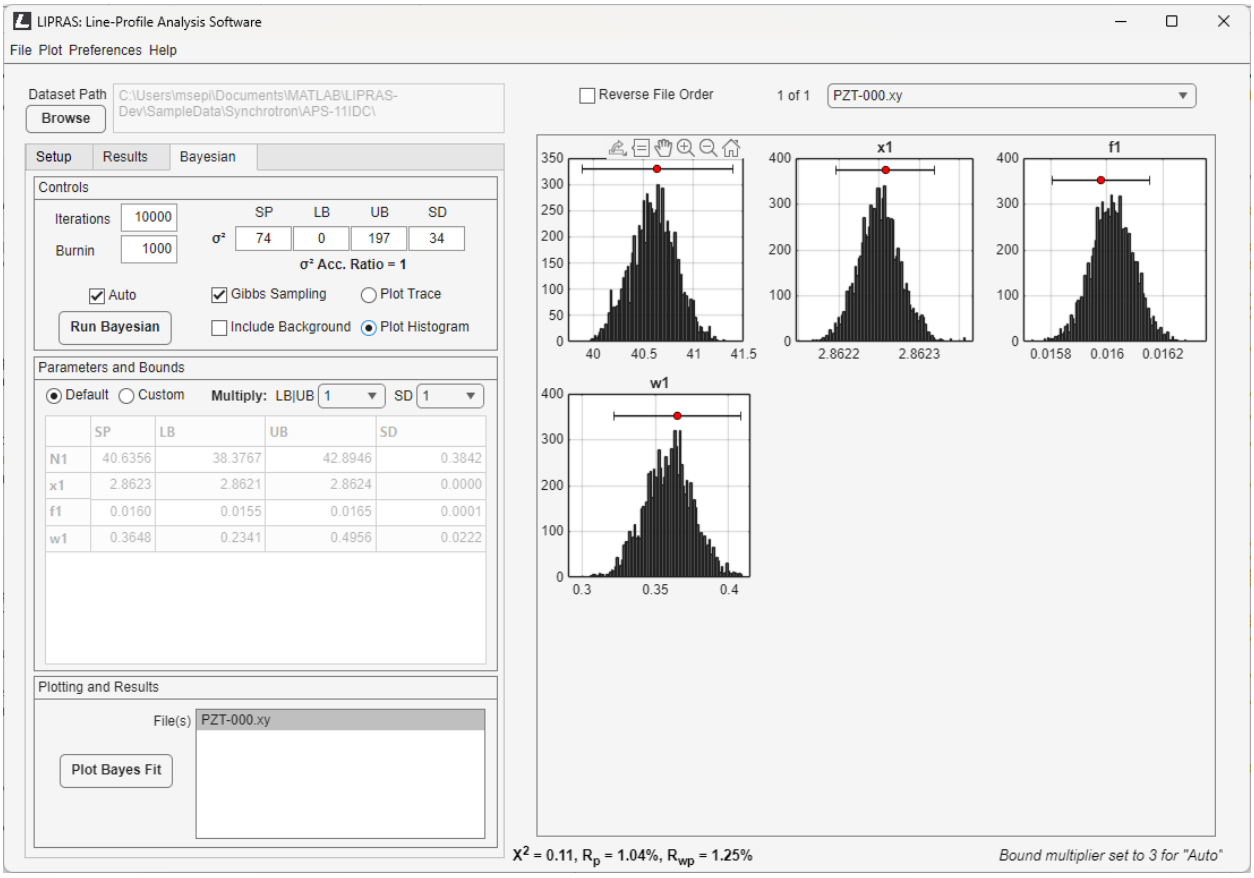
- *Standard Deviation for parameters* is calculated from the 95% confidence interval generated from least squares results and a divider can be selected to enlarge or shrink these for all parameters in the table by using the ‘SD Divider’.

- If you have no idea what you are doing, click 'Auto' and hit 'Run Bayesian'
- Ultimately, all your trace plots for the coefficients should resemble something like:

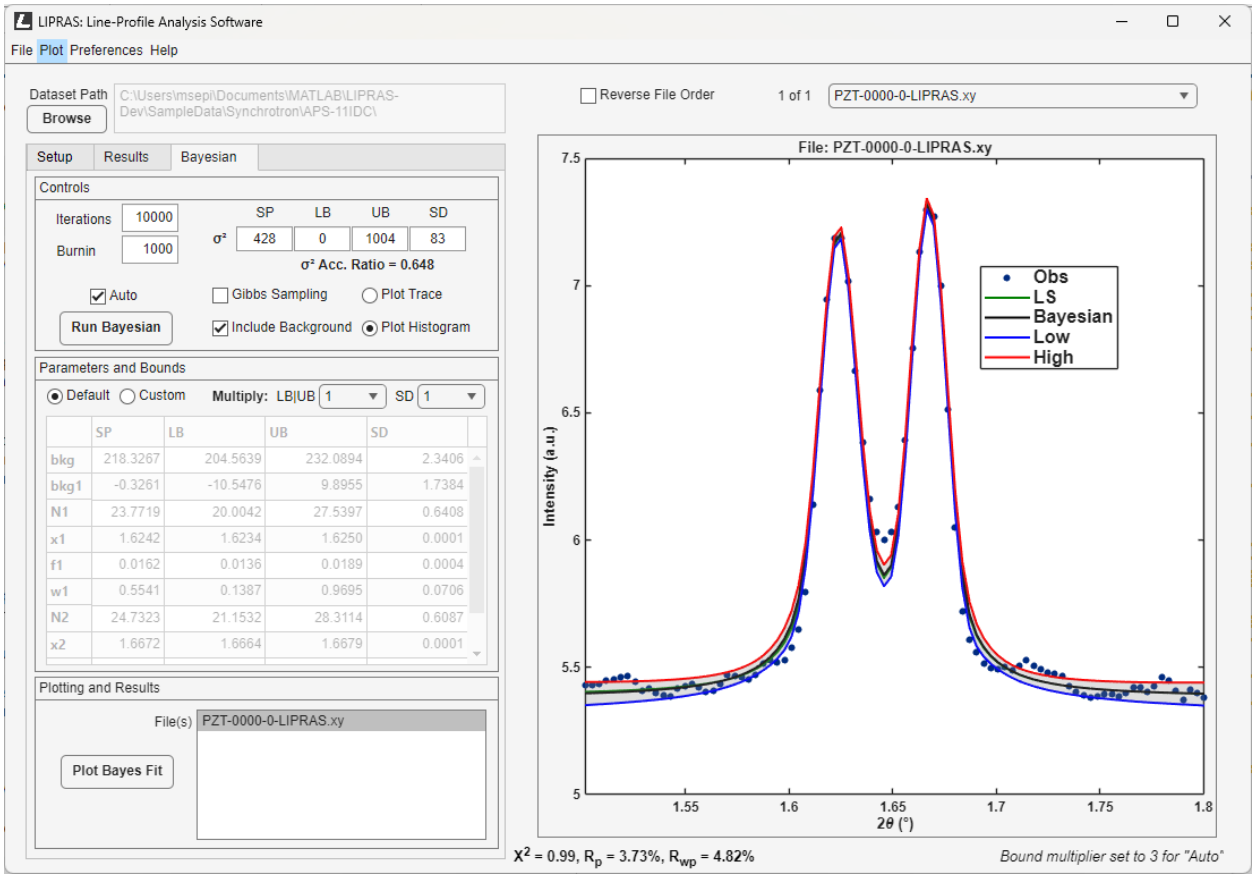


- You can tune σ^2 to determine how log(likelihood) behaves. LogLikelihood is just the log(Eq. 5). It is important to have all your coefficients oscillating around one value.

Histogram plotting for each coefficient describes the posterior distribution



- From here it is easier to see what your mean value is and its corresponding sigma.
    - The red dot with error bars are the least squares results, where the error bars represent the confidence interval.
- All of these results are saved in .BAYES files which contain the fit_mean, the final over all fit, along with its high and low intervals, trace plots of all coefficients, and log(likelihood) which is used to recreate plots such as those shown above.



- The “Plot Bayesian Fit” option displays the Bayesian fit (black) alongside the least squares fit (green), with Rp reported for each. It also overlays the Bayesian 2.5th and 97.5th percentile bounds.
- Selecting multiple files in the list box and hitting ‘Plot Bayes Fit’ will subplot all fits up to 25.

IV. Citing LIPRAS

If you use LIPRAS in your research, please cite it. There is a DOI that has been generated for LIPRAS on ResearchGate, DOI: 10.13140/RG.2.2.29970.25282/3, **click here** to access the technical document associated with this DOI. Citing this document is one of the ways we can measure its success. Lastly, you are welcome to use any of the two following logos for presentations or posters.

Citation, use of the following:

1. Esteves, G., Ramos, K., Fancher, C. M., and Jones, J. L. LIPRAS: Line-Profile Analysis Software. (2017). DOI: https://doi.org/10.13140/RG.2.2.29970.25282/3.

2. Esteves, G., Ramos, K., Fancher, C. M., and Jones, J. L. LIPRAS: Line-Profile Analysis Software. (2017). https://github.com/SneakySnail/LIPRAS.

LIPRAS Logo

V. Obtaining LIPRAS and Updates

LIPRAS is distributed through three sources: MATLAB File Exchange and GitHub for those who wish to use LIPRAS within the MATLAB environment, and SourceForge for those who want a standalone version with no MATLAB dependency. Links are provided by clicking on the bolded text below this paragraph. LIPRAS is open source under a BSD License, which is stated at the beginning of this document. To view the full code, visit the GitHub repository for LIPRAS which is where the code is maintained and updated. To check for updates while using LIPRAS, go to Help> Check for Updates. This prompt LIPRAS to read the HTML page of the GitHub repository and make sure that the version number specified within LIPRAS matches the number of commits in the GitHub repository. If it does, then LIPRAS is up to date. Otherwise, it will prompt the user to go download the latest version by providing the link.

MATLAB Version: [Click Here]
Disclosure: Requires MATLAB® 2023b**,** or higher, Curve Fitting Toolbox™ is recommended by GUI will attempt to run without it.

Standalone Version: [Click Here]
Disclosure: It utilizes MATLAB® runtime which is free and can be downloaded online or through the installation manager.

VI. References

[1] V. K. Pecharsky and P. Zavalij, *Fundamentals of Powder Diffraction and Structural Characterization of Materials*. Boston, MA: Springer US, 2009.

[2] J. E. Daniels, J. L. Jones, and T. R. Finlayson, “Characterization of domain structures from diffraction profiles in tetragonal ferroelastic ceramics,” *J. Phys. D. Appl. Phys.*, vol. 39, no. 24, pp. 5294–5299, Dec. 2006.

[3] A. L. Stancik and E. B. Brauns, “Vibrational Spectroscopy Short communication A simple asymmetric lineshape for fitting infrared absorption spectra,” vol. 47, pp. 66–69, 2008.