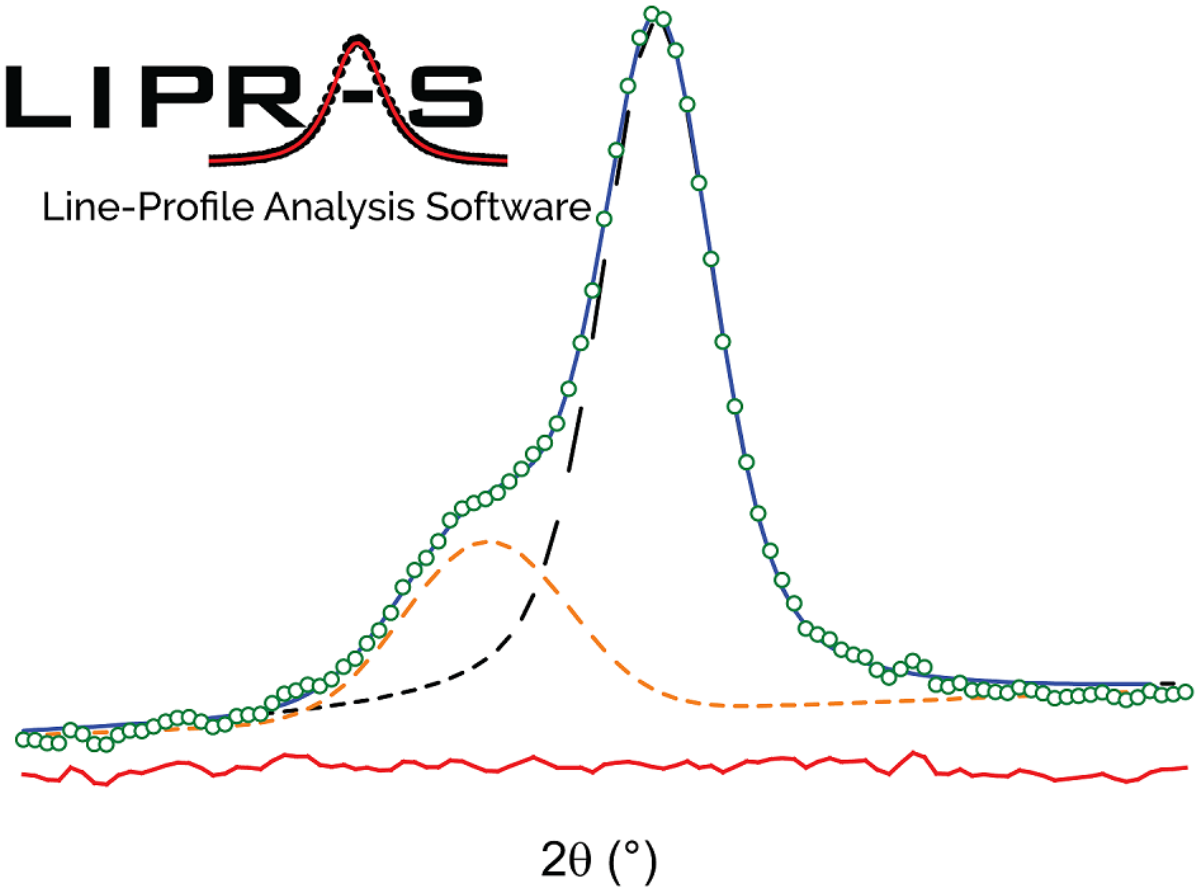
UPDATE NOTES



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April 24, 2017

1. **Functionality:** Exported images are now printed at 100 dpi by default and can be uniquely saved based on preference selection
2. **Functionality:** Export image now creates a separate figure that conducts all plotting and saves it, this prevents unnecessary cycling of the GUI, Export saves the current axes 1 as is, meaning if its zoomed in, it will save the zoomed in region
3. **Bug:** No error message when canceling exporting plot
4. **Stylistic:** Code clean up from GitHub merge conflicts
5. **Stylistic:** Reduced font size on title of plots and statistics plot from 14 to 12
6. **Functionality:** Added the following to Preference tab: Image resolution selection, image format, save all images instead of one
7. **Functionality:** Preference file is now read on start up after all classes have been formed; previously this would happen when a file was read
8. **Functionality:** Preference can now be launched with Ctrl+P
9. **Functionality:** Image export can now be launched with Ctrl+F
10. **Functionality:** When viewing coefficients, export plot will export only that plot and not the fits. Will add Coeffs to the filename as well
11. **Functionality:** Removed 'truesize' command so that Image Processing Toolbox would not be needed to view the about section
12. **Functionality:** (MATLAB Only) On startup save the current directory in case user navigates away and would try to reset LIPRAS
13. **Delete:** Individual Fmodels are no longer written, never had a use for opening one since the master Fmodel contained all the data. The lines were just commented out so MATLAB users can reactivate this whenever
14. **Functionality:** Added individual Kalpha2 peaks to Fdata file. FData now writes peak 1, peak 2, peak… then the Kalpha2 for all peaks

May 19, 2017

IMPORTANT: ***Users who use weights need to ensure they use LIPRAS version 398 or higher.***

LIPRAS version labeling now reflects the commit number on GitHub.

1. **Bug:** Fixed an issue where weights of the first pattern were applied to all the patterns instead of being file dependent
2. **Functionality:** Changed 'Weights' in preference tab to have only [Default, None, 1/obs ($1/\sigma^2$), and 1/sqrt(obs) ($1/\sigma$)]. The 'Default' is for files that have errors associated with measured intensity. To force 1/obs or to have no weights, this must be changed in Weights and can be reverted by going back to 'Default'
3. **Functionality:** Weights for least squares are now written in Fdata
4. **Stylistic:** Rp, Rwp, and GOF (Reduced-χ^2) are now written in the Fmodel file
5. Rp, Rwp, and Reduced-χ^2 are now displayed for each diffraction pattern after a fit below the graphics window
6. **Functionality:** Fdata now prints to 8 decimal places

7. **Functionality:** FXYE and CSV/Excel now reads in the errors columns and sets the weights to the errors in accordance to $1/\sigma^2$. To override, set weights to 'None'
8. **Functionality:** LIPRAS now reads .xye which is twotheta, intensity, error, no header can be present. Errors for these files are set as weights
9. **Bug:** Import parameter file does enable 'Fit Data' when importing
10. **Functionality:** Added feature that can check for updates based on the commits to the master file on GitHub. This is done by reading the html page source and finding the current commit displayed on the GitHub webpage pertaining to LIPRAS
11. **Stylistic:** Interactive help is no longer visible, this requires more work to be useful.
12. **Functionality:** Jacobian matrix from resulting least squares is stored and can be accessed by those using LIPRAS in MATLAB. To do this, type the following into the command Window, after a fit: handles.profiles.FitResults{1}{filenumber}.FitInfo.Jacobian

May 25, 2017

** Commits 415, 416*

1. **Bug:** Fixes to Reduced chi-square, 'Default' weight options for CHI files were incorrect. This was a typo, although could be forced by specifying '1/obs'. Found out GOF or (reduced chi-square) is sse/dfe which are values found in the Fmodel files. In the case of Weights being set to 'None' GOF is calculated the same way as when weights are set to '1/obs'.
2. **Functionality:** LIPRAS assumes sqrt(intensity) for error when reading XRDML files.

June 8, 2017

** Commit 417*

1. **Bug: Significant improvement to background refinement**. Realized that the background needs to be evaluated and modeled with the proper scaling and centering. Therefore, refined model now refines with x=(x-mean(x))/std(x) for the bkg coefficients and is properly evaluated. This change improves the initial guess for bkg coefficients and results drastically. To evaluate the resulting coefficients manually, the x=(x-mean(x))/std(x) must be used.
2. **Stylistic:** Round Rp, Rwp, and GOF to 4 decimal places. For reporting purposes, users should use 2 decimal places.

June 29, 2017

** Commit 418*

1. **Bug:** Added an 'if' statement for when measured intensity was 0, which would cause the weight to be 'Inf' in MATLAB

July 11, 2017

** Commit 419*

1. **Stylistic:** Changed the layout of window of 'Check for Updates' to be more descriptive and display current version and the available version if an update is recommended.
2. **Bug:** Added a try/catch statement to .csv, .xlsx, .xls files for when reading two column data (twotheta, intensity) instead of three column data (twotheta, intensity, error).

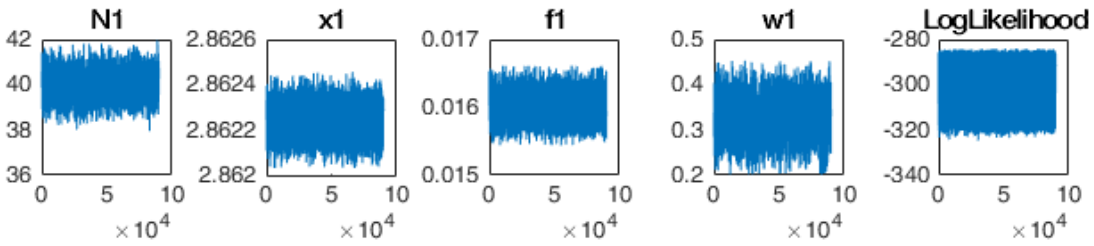
November 6, 2017

** Commit 420*

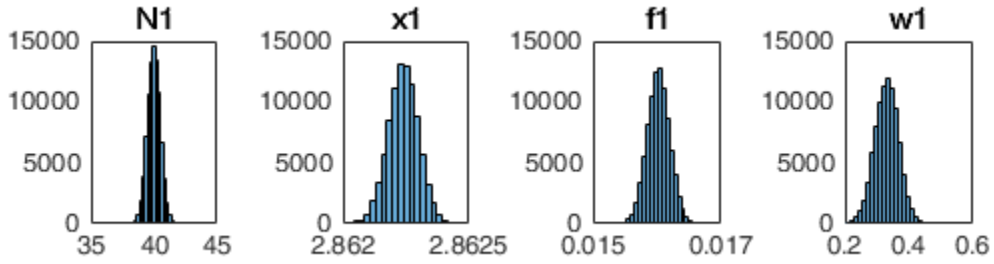
1. **NEW Feature:** Bayesian Inference-***Users need Statistics and Machine Learning Toolbox***, this is an alpha release and may contain errors. Works best on symmetrical functions, asymmetric function can be a hit or miss.
    a. Markov Chain Monte Carlo (MCMC) Metropolis-in-Gibbs Algorithm
    b. This algorithm is explained in https://doi.org/10.1107/S1600576716020057 which is now included in every LIPRAS download.
2. **Bug:** Table would not properly update when the user would hit 'Update' after peak fitting when 'No Bounds' and 'Refine Bkg' were selected and the results led to values that were outside the upper and lower bound. This typically happens when the mixing parameter *w* for the psuedo-Voigt function would result in a value outside of 0-1. Now, the user will have the option to edit the table manually for the values that are excluded.
3. **Bug:** Caused the lower bound of a recently added function to default to the min 2theta. Now, the table should never populate unless peak positions are selected.
4. **Bug:** Fixed an issue that would prevent the user from seeing the adjusted background after changing poly order and hitting 'Update Plot' when 'Refine Bkg' was on. Now, hitting 'Update Plot' without changing poly order and with 'Refine Bkg' ON will do nothing to the Bkg, but once the Poly Order changes and then 'Update Plot' is press then it will calculate a new one and show it. This only applies when changing Poly Order and 'Refine Bkg' is ON, when 'Refine Bkg' is OFF the GUI works as it should.
0. **Functionality:** Table will no longer be editable till peak positions have been chosen
1. **Functionality:** For picking Bkg points, Right-Click now deletes points. Old method should still work, but this will allow people to do everything in one go without having to hit 'Esc'.
2. **Functionality:** On peak position selection, Right-click deletes last point chosen.
3. **Functionality:** LIPRAS changes directory to where .m file is located at launch. This is for those who 'add to path'. Its best if LIPRAS runs while in its current folder.
4. **Functionality:** LIPRAS now checks for updates when launched, if it's up to date then nothing will happen, otherwise, it will notify the user of a new version.
5. **Functionality:** Added a link to LIPRAS manual under 'Help'. This will try to open the local PDF that comes with every download, otherwise, it will open the one in GitHub.
6. **Stylistic:** Constraint coefficients are now italics.
7. **Stylistic:** Default GUI Color is now: White. However, Preference File allows user to change Background color of GUI according to MATLAB's color vector selection: example [0.94 0.94 0.94] is the default [1 1 1] is white, etc. Simply write a new Preference file using LIPRAS and edit the file manually using a text editor.
8. **Stylistic:** Changed text box message during fit to say, "Close this window or minimize to continue working. Press "Cancel" to stop fit."
9. **Addition:** Added csv sample data.
10. **Manual:** Fixed typos

Using Bayesian GUI

- Launch Bayesian GUI
- Table should be populated from results of Least-square refinement, you can change these defaults by switching to 'Custom Bounds'. To Reset any changes, double-click the 'Default Bounds'.
    - Note: If you did peak fitting of multiple files you 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 single file purpose.
    - *Upper bound and lower bound* are determine by taking the difference between the mean value (starting parameter) and the Error*4. The error is just the resulting value minus the reported confidence interval. The multiplier can be changed by MATLAB users, this will be an editable option in a future release.
    - *Standard Deviation for parameters* are calculated from the 95% confidence interval generated from least squares results.
- If you have no idea what you are doing click 'Auto' and hit 'Run Bayesian'
- In the end, you want all your trace plots for the coefficients to resemble something like the following:



- You can tune sigma^2 to determine how log(likelihood) behaves. LogLikelihood is just the log(Eq. 5). However, the important thing is to have all your coefficients oscillating around one value. When you look at the histogram for each coefficient, you get the following:



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