Overview

This application provides a **graphical user interface (GUI)** for analyzing and fitting spectral data. It reads a space-delimited text file containing an x-axis (in the first column) and one or more spectra (in the subsequent columns). The app uses an **Asymmetric Least Squares (ALS)** baseline correction method and **Lorentzian peak-fitting** via **differential evolution**. It fits two distinct peaks (Peak #1 and Peak #2) in each spectrum, then optionally computes a subtraction of the two fitted peaks. You can also save color-coded heatmaps and Excel files with the fitting results.

You now have a **standalone .exe** version, so users can simply run it without needing a Python environment set up.

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Launching the Application

1. Locate the SpectraAnalysis.exe file (or whatever the final name is) on your computer.
2. Double-click the .exe file.
3. The application's main window (GUI) will appear.

If you encounter a **Windows Defender** or **SmartScreen** notice, confirm that you trust this software and click **Run Anyway**.

GUI Layout & Workflow

Theme Selection

1. In the top-left corner of the app, you'll see a **theme selector** (a dropdown menu).
2. Choose a theme (e.g., "arc", "plastik", "clam", etc.). The interface will update immediately to that look-and-feel.

File and Folder Selection

1. In the **"1) File and Folder Selection"** frame, click **Browse** next to **Select .txt File** to pick your spectral data file.
    - The file must be a **space-delimited** text file with the first column as the x-axis and the subsequent columns as individual spectra.
    - Once chosen, the file name will appear in the label.
2. Click **Browse** next to **Select Output Directory** to pick a folder where all results (heatmaps, Excel files, etc.) will be saved.

After you select your .txt file, you'll see an **average spectrum plot** on the right side. This is simply the column-wise mean of all your spectra.

Basic Parameters

In the **"2) Basic Parameters"** frame:

- **Points per Line**: Number of data points per horizontal line (if you want to reshape your data into a 2D map).
- **Lines per Image**: Number of lines (rows) in your 2D map.
    - For example, if you have 110 points per line and 90 lines per image, then one entire "image" or "scan" contains 110 × 90 = 9900 data points, which might match the number of columns or how you intend to visualize your data.

Note: If your data doesn't neatly reshape into this 2D arrangement (because you have more or fewer columns than Points per Line × Lines per Image), the code will gracefully handle it by defaulting to a 1D layout for the resulting arrays.

Peak #1 Definition

In the **"3) Peak #1 Definition"** frame, define the parameters for the first peak:

- **Region Start & Region End**: The x-range over which you want to **baseline-correct** and **fit** Peak #1.
- **ALS lam & ALS p**: Parameters for the Asymmetric Least Squares baseline correction.
    - lam (lambda) is the smoothing parameter (often large: 1e6, 1e7, etc.).
    - p (asymmetry) typically a small fraction near 0 (e.g., 0.001).
- **Mask intervals**: If there are specific x-ranges within this region that **must** be part of the baseline (e.g., areas known to be purely baseline with no signal), enter them here in the format start1-end1, start2-end2, ... For example: 170-175, 327-338.
- **Lorentzian Fit Bounds**:
    - **Position bounds [min, max]**: The expected center of Peak #1. For example, if you believe the peak center is around 245–250, set 245 and 250.
    - **Width bounds [min, max]**: The minimum and maximum allowable Lorentzian width for the differential evolution algorithm.

Click **Preview Baseline Correction (Peak 1)** to open a preview window showing your average spectrum in the selected region, the computed baseline, and how well it fits before you commit to analyzing all data.

Peak #2 Definition

In the **"4) Peak #2 Definition"** frame, define the parameters for the second peak. The same inputs as Peak #1 apply:

- Region start/end
- ALS lam/p
- Mask intervals
- Lorentzian fit bounds (position, width)

Click **Preview Baseline Correction (Peak 2)** if you want to see how the baseline looks on the **average** spectrum for Peak #2.

Subtraction Choice

In the **"5) Subtraction Choice"** frame:

- **Peak1 - Peak2** (option 1)
- **Peak2 - Peak1** (option 2)

The application will compute the difference between the two fitted peaks' **heights**, **widths**, and **centers** based on which radio button is selected.

Save Fitted Spectra

Below the "Subtraction Choice" frame, you'll see a **checkbox** labeled **"Save Fitted Spectra"**.

- If checked, the program will generate and save **individual .png** plots showing each spectrum's raw data, baseline, and fitted Lorentzian for both Peak #1 and Peak #2.
- These plots will go into a subfolder named **Fitted_Spectra** within your chosen output directory.

Analyze Full Data

Finally, click the **"Analyze Full Data"** button:

1. The code will iterate over all columns (spectra) in your file.
2. Perform ALS baseline correction and Lorentzian fitting for Peak #1.
3. Perform ALS baseline correction and Lorentzian fitting for Peak #2.
4. (Optional) Generate and save each **Fitted Spectrum** plot if you checked that box.
5. Reshape the results into 2D arrays (according to Points/Line and Lines/Image) or leave them 1D if they don't reshape neatly.
6. Produce **heatmap** images (.png) for:
    - Peak #1: Height, Width, Center
    - Peak #2: Height, Width, Center
    - Their differences (Height Diff, Width Diff, Center Diff)
7. Save all numeric results into **Excel** files (.xlsx), including separate Excel files for each peak's raw results and one for the difference.

A **Progress Bar** shows the progress of the analysis (each spectrum requires 2 fits: Peak #1 and Peak #2).

Results and Output Files

1. **Subfolders** in your chosen output directory:
    - **Peak1_[avgC1Value]**

        - Contains Peak1_Height.png, Peak1_Width.png, Peak1_Center.png, and an **Excel** file (Peak1_results.xlsx) with columns [Height, Width, Center].
        - The [avgC1Value] in the folder name represents the **average peak center** for Peak #1 across all spectra.
    - **Peak2_[avgC2Value]**
        - Contains Peak2_Height.png, Peak2_Width.png, Peak2_Center.png, and an **Excel** file (Peak2_results.xlsx) with columns [Height, Width, Center].
        - The [avgC2Value] in the folder name represents the **average peak center** for Peak #2 across all spectra.
    - **Substraction**
        - Contains Height_Diff.png, Width_Diff.png, Center_Diff.png, and Difference_results.xlsx with columns [HeightDiff, WidthDiff, CenterDiff].
2. If **"Save Fitted Spectra"** was checked, you'll also see:
    - **Fitted_Spectra** subfolder:
        - Contains .png files for each spectrum, named peak1_spectrum_0001.png, peak2_spectrum_0001.png, peak1_spectrum_0002.png, etc.
        - Each image shows the original data, baseline, and Lorentzian fit for the specified peak.

Troubleshooting and Tips

- **No File Selected**: You must pick a .txt file first. If no file is selected, you'll see a warning message.
- **Points/Line & Lines/Image**: Make sure these integers multiply to the number of spectra you have, if you want meaningful 2D heatmaps. Otherwise, the code will still work, but the 2D reshape will fall back to a 1D layout.
- **Mask Intervals**: If you don't need any forced baseline regions, you can leave it empty.
- **Lambda (lam) and p**: Larger lam yields a smoother baseline. Adjust p around 0.001 – 0.01 to see how it affects the asymmetry.

- **Bounds**: Make sure your pos and width bounds are sensible for the data. If the algorithm fails to converge or the results look strange, try broadening the bounds or updating maxiter inside the code (though the default is usually sufficient).
- **Differential Evolution**: This algorithm can be slow if your dataset is very large. Monitoring the progress bar is helpful.
- **Errors**: If you see an unexpected error message or the program stops, double-check your input fields for valid numeric values.

Thank you for using the Spectra Analysis Application!
If you have further questions, feel free to reach out.