Your Report Title

Your Name

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Abstract

Your abstract goes here.

1 Introduction

1.1 Signal Preprocessing

1.1.1 Whittaker Smoothing vs. Asymmetric Least Squares (AsLS) for Spectroscopy

Whittaker smoothing is a classic method for smoothing data, formulated as a minimization problem:

$$\min_z \sum_i (y_i - z_i)^2 + \lambda \sum_i (D^2 z_i)^2$$

where y is the observed signal, z is the smoothed signal, D^2 is the second difference operator, and λ controls the trade-off between fidelity to the data and smoothness. Whittaker smoothing is linear, treats positive and negative residuals equally (symmetric), and has a single trade-off parameter λ. The solution is closed-form.

Asymmetric Least Squares (AsLS) modifies only the data fidelity term by introducing weights:

$$\min_z \sum_i w_i (y_i - z_i)^2 + \lambda \sum_i (D^2 z_i)^2$$

where $w_i = p$ if $y_i > z_i$ and $w_i = 1 - p$ if $y_i < z_i$, with p typically close to zero. The weights depend on the current solution z, making the problem iterative and asymmetric. AsLS actively ignores peaks by down-weighting positive residuals, focusing on fitting the lower envelope of the signal—ideal for baseline removal in spectroscopy.

In AsLS, λ is typically chosen by heuristics (e.g., $\lambda \sim 10^4$–10^8 for spectroscopy) and visual inspection. In summary, AsLS uses Whittaker as a subproblem but adds asymmetric, adaptive weighting, making it more suitable for baseline correction in spectroscopy.

1.1.2 Low-pass filter

For removing high-frequency noise from Raman spectra, a Butterworth low-pass filter is used.

1.1.3 Normalization

Min-max normalization rescales every spectrum to the same range, typically [0, 1], using the formula:

$$x' = \frac{x - x_{min}}{x_{max} - x_{min}}$$

where x is the original value, x_{min} and x_{max} are the minimum and maximum values of the spectrum, and x' is the normalized value.

However, in Raman, peak intensity carries chemical information. Thus, using min-max normalization amplifies noise and baselinea artifacts. Instead, standard normalization (z-score normalization) is preferred:

$$x' = \frac{x - \mu}{\sigma}$$

2 Methods

Describe your methods here.

3 Results

Present your results here.

4 Discussion

Discuss your findings here.

5 Conclusion

Summarize your conclusions here.