Supervised Machine Learning for Post-Acquisition Background Suppression in Tip-Enhanced Raman Spectroscopy (TERS)

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Tip-Enhanced Raman Spectroscopy (TERS) is a chemical imaging technique that enhances weak near-field Raman signals to map the composition, structure, and physical properties of materials between 1-10 nanometers. These signals are often obscured by strong background contributions such as fluorescence, elastic scattering, and instrumental noise. This work presents a post-acquisition framework for suppressing background signals while preserving chemically meaningful Raman peaks. Raw arrays were smoothed using a Savitzky-Golay filter, and MATLAB's findpeaks algorithm with sensitivity-tuned parameters generated an overcomplete set of candidate peaks. Peak features, including prominence, symmetry, and height, were extracted and used to train a random forest classifier on manually labeled peaks to distinguish true Raman peaks from noise. A slope based boundary algorithm then suppressed all non-peak spectral regions, substantially reducing background noise. The classifier achieved an average F1 score of 0.929 with only 300 manually labeled peaks, suggesting that expert labeling would likely push performance higher. The peak-only output produced the strongest spatial contrast and most effective background suppression among all methods compared, including Asymmetric Least Squares. Peak shift analysis showed shifts were centered around 0 cm^-1, never exceeding 6 cm^-1 (<30% of half FWHM), consistent with Savitzky-Golay smoothing and within an acceptable range for chemical interpretation. The classifier can be quickly retrained with minimal labeled data without redesigning the pipeline, demonstrating that machine learning and signal processing can meaningfully complement physical measurement techniques and offer a cost-effective alternative for background suppression in TERS.

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