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Chemometrics-driven data acquisition to accelerate confocal Raman imaging

In time-sensitive applications such as Raman spectral imaging, the conventional workflow where chemometric analysis is deferred until after full data acquisition is increasingly being challenged. Could one actually make a decision before the completion of the full « brute-force » acquisition? This would open up possibilities to optimize experimental throughput and accelerate the analysis.

In this regard, within the framework of linear spectral unmixing, we have developed a strategy that relies on the early (low SNR) detection of essential spectral pixels -those exhibiting maximal linear dissimilarity- followed by targeted high-SNR measurements at these critical locations. Such an adaptive sampling approach has recently been shown to accelerate acquisition time by at least one order-of-magnitude while inducing negligible information loss.

The proposed approach is grounded upon two key transformations of the raw spectral data: i) their L_1 -normalization, addressing the dual challenge of compositional geometry in mixture systems and SNR optimization, and ii) their discrete Fourier transform, which can be computed spectrum by spectrum for real-time adaptability.

References

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