Chemometrics and Machine Learning in Raman Spectroscopy

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As a label-free technology, Raman spectroscopy has become extremely appealing in biological and clinical applications for diverse tasks including microbial identification and disease diagnosis. Its power by large owes to and is enhanced by machine learning and chemometric approaches, in which chemometric and statistical models are constructed to extract and translate the Raman signal of interest into high-level biological or clinical knowledge. The presentation will walk through the key steps of Raman data analysis, ranging from experimental design to spectral preprocessing, from model construction to evaluation. We will provide our experience and insights on the pitfalls, open issues, and possible solutions in Raman spectral analysis. Additionally, the concepts and approaches of model transfer will be introduced along with our latest research and results.

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