

Spectral Component Analysis

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Abstract: New method for variance decomposition of near-infrared spectra is summarized. It hybridizes pre-processing with classical decomposition methods (exemplified through Principal Component Analysis). It combines subtraction of the closest solvent spectrum [1] and additional spectra of the main chemical components of the sample. Since only subtraction is used:

1. Calculation and results are straightforwardly interpreted.
2. Physical units of measurement are retained.
3. Lower computational costs are maintained.

Proposed procedure is applicable to chemical systems whose main components are known or can be deduced. It is advantageous since:

1. Variance is splitted in a variable-correlated manner which closely corresponds spectral variance.
2. Bands are visualised and variables automatically selectable (visualized peaks).
3. Functional as well as statistical methods can now be applied.

Comparison with Principal Component Analysis reveals advantages, challenges and distinctive features.

References

- [1] Kojić D. Tsenkova R. Yasui M., *Anal. Chim. Acta*, 2017, 955, 86-97.