A Poor Man's Guide to AquaPhotomics: Analysis of Variance in Near-Infrared Spectra of Water.

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November 19, 2018

Abstract: A different outlook on variance decomposition in near-infrared spectra is presented. Spectra of pure water are perturbed with respect to pathlength and temperature to demonstrate how each position to the right of the decimal point (orders of magnitude) corresponds to relevant physical properties of water. Physical properties are linked to chemical properties of aqueous solutionsto show how:

1. Changes in **pathlength** generate the largest amount of variations, located at the first decimal point.
2. Changes in **temperature**, localized around two main sub-bands (1412/ 1492 nm) generate variation at the second decimal point.
3. **Hydrogen bonds** can change their strength in response to (mainly) temperature and molecular composition (self-dissociation, solutes, etc.), and occur at three sub-bands, thus generating variation at the third and fourth decimal point.
4. **Charge transfer** affects the short wavelength region (1100-1370 nm) that receives influences from the neighbouring visible region (400-800 nm) due to self-dissociation, partial/full charge transfer from solutes, and generates variation at the remaining decimal points ($\geqslant$5).

Since decomposition is performed simply by subtraction: (1) computation is straightforward, (2) physical units of measurement are retained, and (3) low computational costs are maintained. Comparison with PCA reveals advantages, challenges and distinctive features.

References

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