Workshop

Removing Interference Signal from NIR Spectra

Ali Gahkani

Aunir, Towcester, United Kingdom

In this workshop, the concept of pre-whitening aquaphotomics data will be explored using a practical example. An interference matrix derived from repeated NIR measurements of identical samples under varying ambient conditions will be used to down-weight the influence of such interferent factors on subsequent data analysis. EPO (External Parameter Orthogonalization) and GLSW (Generalised Least Squares Weighting) will be used as two related approaches in this context.

Eigenvector Solo software is a pre-requisite for this workshop. Please download a fully functional 30-day demo version of Solo before attending: http://www.eigenvector.com/software/solo.htm

Invited talk

Covariance Weighting in Aquaphotomics

Ali Gahkani

Aunir, Towcester, United Kingdom

Robustness and transferability of any aquaphotomics solution is highly dependent on devising an effective strategy to eliminate the influence of interferent signals from the NIR spectra. Such interfering factors could be ambient, chemical and instrumental in nature and are often difficult to control or standardise. To tackle this problem spectral pre-processing methods such as spectrum subtraction, normalisation and scatter correction have been proposed in the past.

In this work, first time application of a covariance weighting approach called GLSW[*] (Generalised Least Squares Weighting) in aquaphotomics is presented and its effectiveness in quantification and classification is demonstrated using a competition dataset[**]. The difference between spectra of identical samples measured under varying external factors is called a covariance matrix (also known as interference matrix or clutter).

GLSW is easy to apply and provides a greater flexibility when compared to related methods such as EMSC (Extended Multiplicative Scatter Correction) and EPO (External Parameter Orthogonalization).

[*]*Martens, Harald, et al. "Pre-whitening of data by covariance-weighted pre-processing." Journal of Chemometrics: A Journal of the Chemometrics Society 17.3 (2003): 153-165.*

[**] *2018 IDRC software shoot-out"*