Abstract

Orthogonalisation techniques for correcting temperature, scattering, moisture and instrument effects

Fabien Chauchard[1], Sébastien Preys[2], Jean-Michel Roger[3], Juan Antonio Fernandez Pierna[4], Pierre Dardenne[4] and Sylvie Roussel[1,2]*

[1]Indatech, SAS, 385 avenue des Baronnes, 34730, Prades-le-Lez, France
[2]Ondalys, SARL, 385 avenue des Baronnes, 34730, Prades-le-Lez, France
[3]Cemagref, UMR Information and Technologies for Agro-Processes, BP 5095, 34033, Montpellier, France
[4]Walloon Agricultural Research Centre (CRA-W), Quality of Agricultural Products Department, Chaussée de Namur no. 24, B-5030, Gembloux, Belgium
*Corresponding author: sroussel@ondalys.fr

Introduction

Multivariate calibration of NIR spectrometers generally relies on a linear model which is particularly sensitive to even small changes in the spectra. Thus, the prediction performances can be dramatically altered by a lot of influencing factors, such as temperature, particle size, moisture or instrument. In order to deal with potential lack of robustness, several approaches have been proposed. The usual approaches integrate all possible effects of influencing factors into the calibration database. The main drawback of this approach is the resulting large number of calibration samples to be measured (spectra and reference values). For this reason, some orthogonalisation methods have been proposed, such as External Parameter Orthogonalisation (EPO), Transfer by Orthogonal Projection (TOP) and, more recently, Orthogonal Signal Correction (OSC) with experimental design. These methods aim at identifying the subspace of perturbation using few samples (only spectra) to remove it from the calibration database.

Materials and Methods

This work presents a complex application in which several perturbations have to be removed in order to build a robust model, having at hand only 10 calibration NIR spectra with the corresponding reference values and several experimental designs (only spectra) containing the different perturbation information. This study stems from a real application and is the result of the “Chimiométrie 2007” conference shootout. Three orthogonalisation techniques were implemented, i.e. EPO, an approach based on exhaustive calibration with a synthetic database, and OSC with this synthetic database.

Results and Discussion

Each of the 3 approaches gave interesting results by significantly improving the calibration model robustness. The approach using the synthetic database gave the best R^2, EPO the best RMSEP and bias and knowledge about the removed perturbations, and OSC the least noisy b-coefficients and knowledge about the removed perturbations as well.

Conclusion

Experimental knowledge can be used to improve the robustness of calibration models and orthogonalisation techniques show promising results to handle perturbations identified by small experimental designs.

Reference paper as:
F. Chauchard, S. Preys, J. Roger, J. Fernandez Pierna, P. Dardenne and S. Roussel (2012). Orthogonalisation techniques for correcting temperature, scattering, moisture and instrument effects (abstract), in: Proceedings of the 15th International Conference on Near Infrared Spectroscopy, Edited by M. Manley,C.M. McGoverin, D.B. Thomas and G. Downey, Cape Town, South Africa, p. 130.