Research on orthogonal signal correction in near infrared calibration

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Introduction

There is no denying that OSC is effective in reducing signals which are orthogonal to the property of interest; nevertheless, the suitable use of OSC has not been found in NIR applications yet. This paper aims to investigate the problem of OSC in application and to take full advantage of OSC in NIR modeling.

Materials and Methods

Samples used in this paper include honey, blending edible oils, and dimethylsulfoxide solution. A SupNIR-5500 near infrared spectrometer (Focused Photonics Inc) was used over the wavelength range 1100 to 1800 nm (6nm resolution) with a 2 mm pathlength. Data processing was carried out in MATLAB 7.0 (Mathworks, Inc) and chemometric software CM-2000 (Focused Photonics Inc).

Results and Discussion

The external validation results of MLR models using OSC and of PLS1 models were as follows: Peanut oil in binary blending edible oil (v/v, %): PLS1 R_p=0.9997, SEP=0.61; OSC+MLR R_p=0.9998, SEP=0.61. Peanut oil in tertiary blending edible oil (v/v, %): PLS1 R_p=0.9997, SEP=0.66; OSC+MLR R_p=0.9998, SEP=0.59. Dimethylsulfoxide (w/w, %): PLS1 R_p=0.999992, SEP=0.109; OSC+MLR R_p=0.999996, SEP=0.094.The linearity between spectra and property and the symmetry of mean centered spectra is very helpful to determine the best OSC component number. Although OSC + PLS can improve the results of cross-validation markedly, it cannot improve the results of external validation, even making them worse. A combination of OSC with MLR can greatly improve the predictive power of the calibration model, with the results obtained being even superior to that of a PLS1 model.

Conclusion

Application of OSC to PLS modeling brings about over-fitting. The predictive power of models is greatly improved by a combination of OSC with MLR. The performance of an OSC +MLR model is superior to that of the PLS1 model.

Reference paper as:
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