Abstract

PLS algorithms and variants including LOCAL applied to natural products

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Introduction

The linear methods PLS and MPLS, and the non-linear methods LOCAL and ANN are often used in NIR spectrometry. Non-linear methods can result in one single application for wide ranges of samples, with accuracies as good as or better than what is obtained from a set of separate linear models. Another topic is regarding different PLS algorithms. Their differences in prediction are small but fundamental mathematical properties like the underlying orthogonality differ. Until recently, there was no objective method to compare them.

Materials and Methods

All instruments were from FOSS of Hillerod, Denmark. Soybean extracts containing 16-93% protein were analyzed with an Infraxact (570:0.5:1848 nm). PLS, MPLS and LOCAL calibrations were created from all 1202 samples using the WinISI calibration package. A test set with new samples analysed afterwards was used to evaluate the performance. In a different study, nine PLS algorithms were compared using data sets from the food and pharmaceutical area. The instruments used were NIRSystems 6500 (400:2:2498 nm), Milkoscan FT120 (923:3.8:5012 cm^{-1}) and Infratec 1241 (570:2:1098 nm).

Results and Discussion

It was found that the SEP(MPLS) = 0.9% was slightly better than SEP(PLS) = 1.0%. This improvement is similar to what has been found also in other studies. The SEP(LOCAL) = 0.6% was the best due to the heterogeneity of the samples, with the important additional benefit of simplicity for the operator of having only one application to choose from. This system is now fully implemented in industry. In the other study, NIPALS, the non-orthogonalised scores algorithm, improved kernel PLS, direct-scores PLS1 all showed excellent mathematical properties. The two last resulted in ~4 times faster calibration calculations.

Conclusion

LOCAL resulted in one single application to choose from and a superior SEP. PLS algorithms based on deflation were found to have the best mathematical properties.

Reference paper as:
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