Abstract

Comparison of various chemometric evaluation approaches for near infrared spectroscopic data of feed and feed products

J.A. Fernández-Pierna,[a] B. Lecler,[a] J.P. Conzen,[b] A. Niemoeller,[b] P. Dardenne[a,*] and V. Baeten[a]

[a]*Walloon Agricultural Research Centre (CRA-W), Quality of Agricultural products Department, Chaussée de Namur 24, Gembloux B-5030 Belgium. E-mail: dardenne@cra.wallonie.be*

[b]*BRUKER OPTIK GmbH, NIR & Process Technology, Rudolf-Plank-Str. 27, Ettlingen 76275 Germany*

Introduction

In most of the countries that produce important amounts of feed, feed ingredients, fresh silages or soil products, regulations and laws exist to control the chemical composition of these products. Normally these regulations specify some limits (minimum water content, etc.) in the final product, in order to guarantee that it meets their legitimate expectations and fulfils good manufacturing practice. However, manufacturers want to produce at minimal costs, so they try to arrange their formulations so that the chemical composition of the products approaches the limiting values. In order to do so, the chemical composition of the raw materials must be known accurately. This requires considerable analysis, involving analytical methods which are expensive, and require the use of reactive chemicals. Near infrared (NIR) spectroscopy is a useful alternative to these analytical techniques. It is the most widely used non-destructive technology in the feed industry, and is an official control method to determine qualitative parameters of feed ingredients and feeding stuffs. The high throughput of the method, the capacity to determine in one single analysis a large panoply of parameters, and the possibility to build networks of spectrometers made this technique very attractive for the feed sector. The fact that the method can also be used on-line in a feed production plant made this technique even more attractive. The objective of this work was to compare the performance of different supervised regression methods, based on NIR data of feed, feed ingredients, fresh silages and soils for the prediction of several properties.

Materials and methods

Spectral data of four different products and different properties for each were available: (1) Feed: ash, fat, fibre, starch, protein; (2) Feed ingredients: ash, fat, fibre, protein; (3) Fresh silages: dry matter, fibre, protein and (4) Soils: CEC (cation exchange capacity, COT_SK (organic carbon), N_Kj (nitrogen).

Results and discussion

A regression model for each property and for each data set was determined, which can then be applied to classify new (unknown) samples. A full analysis including diagnostics, feature reduction/selection, modelling and validation of models was performed. Chemometric models were constructed using PLS, ANN and LS-SVM. LS-SVM gives similar results than ANN but in most of the cases its prediction ability is higher than the other two methods (lower RMS Errors). In most cases, PLS gives poor results, in some cases this can be due to the fact that the relationship between the predicted values and the actual concentration is not linear. This can be checked by visual examination of the method response versus the analyte concentration. This usually works well, but it is subjective and open to different interpretations. The results show that in general, ANN and LS-SVM are very powerful methods for non-linearity. but LS-SVM is also performing quite well in the case of linear models.