

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

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Introduction

In most of the countries that produce important amounts of feed, feed ingredients, fresh silages or soil products, regulations and laws exist about the chemical composition of these products. Normally these regulations lay down some kind of limits (minimum water content, etc) in the final product in order to guarantee that it meets their legitimate expectations and fulfils the good manufacturing practice. However, manufacturers want to produce at minimal costs and try to arrange their formulations in a way, that the chemical composition of the products is approaching those limiting values. In order to do so, the chemical composition of the raw materials must be known. This requires considerable analytical methods, which are expensive and require the use of chemical reactive.

The objective of this work is 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.

Material and methodology

NIR spectral data (measured in the range 1100:2500 nm and a resolution of 2 nm) with reference values of different properties for four different products were used:

- **Feed:** Ash, Fat, Fibre, Starch, Protein (28676 spectra)
- **Feed Ingredients:** Ash, Fat, Fibre, Protein (26652 spectra)
- **Fresh Silages:** Dry Matter, Fibre, Protein (1035 spectra)
- **Soils:** CEC (Cation Exchange Capacity, COT_SK (Organic Carbon), N_Kj (Nitrogen) (1625 spectra)

The spectral data were pre-processed by the Standard Normal Variate transform followed by detrend and 1st derivative Savitzky-Golay treatment (15,2,1) in order to remove the scattering effects and to smooth the spectra.

A regression model for each data set and for each property is determined, which can then be applied to predict new (unknown) samples. A full analysis including diagnostics, feature reduction/selection, modelling and validation of models has been performed.

Chemometric models have been constructed using PLS¹, ANN² and LS-SVM³.

NIRS is the most widely used non-destructive technology in the feed industry and 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 large panoply of parameters and the possibility to build network of spectrometers made this technique very attractive for the feed sector. The fact that this method can be also used on-line in a feed production plant made this technique even more attractive.

For the application of all the different regression methods, the data set is split into three subsets. The one used for model construction constitute the *training set* (80% of the samples). The models obtained using this training set are then applied to *two test sets* (10% of the samples each). These two test sets have been selected in two different ways: by using the duplex design proposed by Snee⁴ (*ks set*) and randomly (*rd set*). Samples selected by the duplex method cover the whole range in the PC space. The random selection contains less extreme samples than the test selected by duplex.

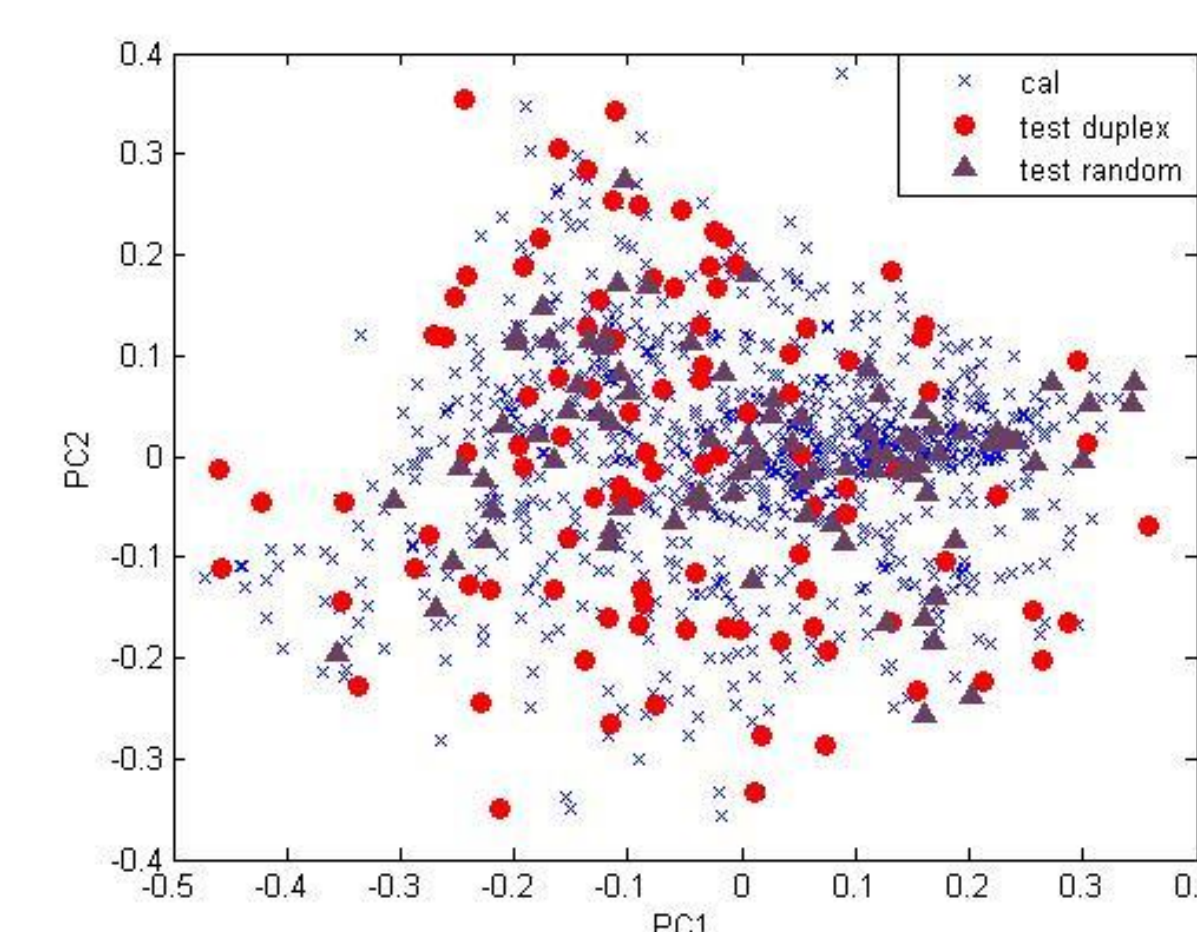
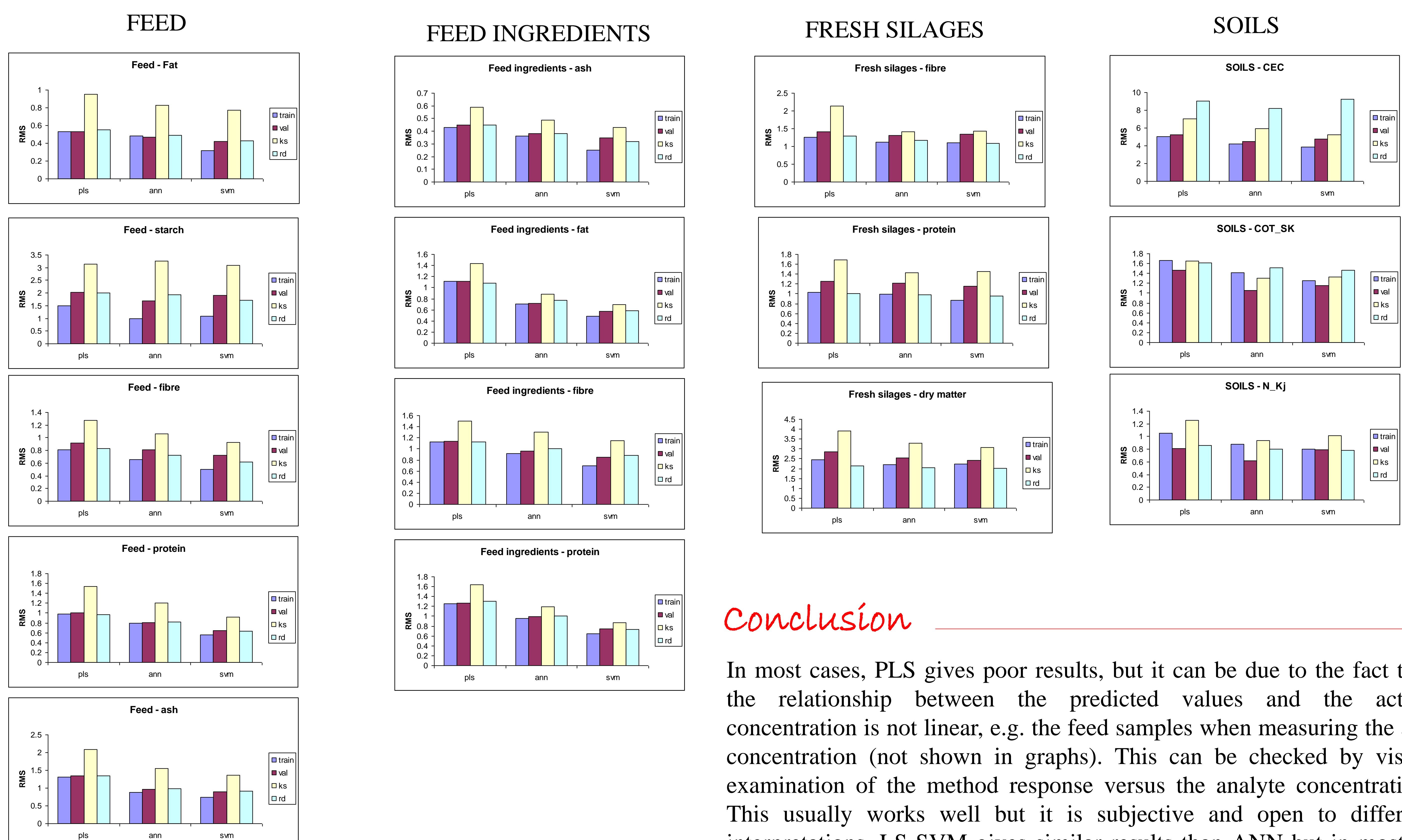


Figure 1 – Samples selected using the duplex method

Results



Conclusion

In most cases, PLS gives poor results, but it can be due to the fact that the relationship between the predicted values and the actual concentration is not linear, e.g. the feed samples when measuring the ash concentration (not shown in graphs). 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. 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).

LS-SVM gives in general better results not only for clear non-linear cases, but also is performing quite well in the case of linear models.

References

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