Development of global near infrared transmission calibrations for moisture and protein in cereals using artificial neural networks and very large data sets

Nils Bo Büchmann
DLG (Danish Cooperative Farm Supply), Axelborg, DK-1603 Copenhagen V, Denmark.
E-mail: nbb@dlg.dk.[*]

Introduction

Until recently, near infrared (NIR) transmittance measurements of protein and moisture in wheat, barley and other cereals, using Foss Tecator Infratec instruments, were based on partial least squares (PLS) calibrations which, typically, were developed using a couple of hundred samples. In 1995, the present author proposed, as an alternative, the use of artificial neural network (ANN) mathematics and very large data sets.[1] All the European NIR transmittance networks in existence at that time provided data for the project and these ANN calibrations have been in commercial use in several European networks for three years. As reported elsewhere,[2] the ANN calibrations have proved to be very accurate, notably at extremely high moisture levels, where PLS models fail. The common European models are also superior with respect to transferability and stability.

The common European model for moisture has been tested with cereal samples from other continents. Prediction results from a set of North American wheat and barley samples, measured by the National Testing and Evaluation Programme (NTEP), are presented below as an example. It will be concluded that the European ANN model for moisture is already globally applicable. (The term "global" is used here in its literal sense).

To develop a similar global calibration for protein in wheat and barley, key Infratec users in Australia and North America transferred their Infratec data files to Foss Tecator, to be combined with the European data set. The total data set then consisted of 28,102 samples. To the knowledge of the present author, a data set of this size has never been used before for calibration purposes. The accuracy of the resulting global ANN model for samples from all three continents will be evaluated in this paper. Also, the experiences, from a practical point of view, of using ANN mathematics over linear models will be briefly discussed.

[*]Address at the time the study was presented.
Current address: Foss Tecator AB, Box 70, SE-26321 Höganäs, Sweden. E-mail: bo.buchmann@foss.tecator.se.

Materials and methods

Participating networks

The European networks (listed below in alphabetic order) are all members of the common European Grain Network Group and have kindly provided data from the 1991 to 1998 harvests to Foss Tecator for the development of the European and global ANN models:

- **Agronet**, Sweden
- **Doemens**, Germany
- **GIEI**, France
- **Raiffeisen Nord**, Germany
- **RWA** (Raiffeisen), Austria
- **Station de Haute Belgique**, Belgium
- **The National Network**, Denmark
- **The National Network**, England & Scotland
- **Ulice' Infratec Network** (Limagrain), France

The two North American participants kindly agreed to provide data sets for the development of the global calibration model for protein in wheat and barley. This commitment does not oblige the two North American agencies to use the resulting ANN models in practice:

- **GIPSA** (Grain Inspection, Packers and Stockyards Administration, US Dept. of Agriculture), United States of America
- **CGC** (Canadian Grain Commission), Canada

GIPSA also provided the samples for the intercontinental ring test.

The Australian participant is currently using an Australian ANN protein and moisture model for wheat and barley:[3]

- **CBH** (Co-operative Bulk Handling Limited (CBH), Western Australia), Australia

Reference method

At the time the data were compiled (autumn 1998), all the participating North American and European reference laboratories were using the Kjeldahl method for determining protein. The Australian reference laboratory used both Kjeldahl and combustion (LECO). All laboratories used the oven drying method for moisture. To allow comparison between laboratories, all protein results were recalculated to a dry matter basis regardless of local practices. Based on the results from a European ring test, the protein reference values for the European samples were harmonised to a common level; the reference values were not otherwise adjusted.

Intercontinental ring test

A set of 20 samples of Hard Red Spring wheat from North America were subdivided and distributed to 18 Australian, European and North American laboratories by GIPSA in October 1998. All nitrogen values were multiplied by 5.7 and the protein content corrected to dry matter. Two of the European laboratories received insufficient sample material to allow measurement of both protein and moisture; in these two cases moisture values from another European laboratory were used for moisture correction.

Table 1. Origin and use of the data set of wheat and barley samples used to develop the global ANN calibration model WBP18.

Commodity	Training set	Stop set	Test set
Australian wheat	37%	38%	28%
Australian barley	14%	16%	10%
European wheat	14%	12%	21%
European barley	13%	10%	21%
North American wheat	21%	23%	19%
North American barley	1%	1%	1%
Total number	16.796	4.944	6.362

Origin and use of data sets

The origin and use of the data set used to develop the global ANN model for protein in wheat and barley, WBP18, is summarised in Table 1.

The data set represented approximately 30 different sub-masters of Infratecs types 1221, 1225 and 1229. Instrument stabilisation scans, measured with deliberate monochromator errors, were also included. Finally, scans from very warm and cold samples were added to improve temperature stability. The samples themselves were from 1987 to 1998 and represented a very broad variation with respect to climatic conditions and variety. Approximately 7% of the samples were durum wheat and all the major North American wheat classes were represented.

A very large number of sample sets were set aside to allow prediction on sizeable subsets representing a particular class or data from a particular country.

The ANN calibration model WBMO5 for moisture in cereals was used for the NTEP-testing of moisture in American 6-row barley. This model is based on European samples of wheat, barley and oats.

Development of the calibration models

Samples with absorbance levels above 5 OD were excluded from the data set and the 2nd derivative of the NIR transmittance scans was used for a subjective elimination of erroneous scans. In total, less than 1% of the data set was discarded. The remaining NIR transmittance scans were subjected to a proprietary preprocessing before ANN calibrations were developed using back propagation. Both WBMO5 and WBP18 models were developed by Foss Tecator.

Statistics

The accuracy of the predictions was evaluated by means of the bias and the standard error of prediction (*SEP*). Furthermore, the ratio of standard error of prediction to standard deviation (*RPD*) was calculated as the standard deviation in the population of the samples predicted divided by the *SEP* for the same prediction set; the *RPD* being a ratio is dimensionless.

Table 2. Prediction statistics for moisture and protein in wheat and barley samples from Australia, Europe and North America using the European ANN moisture model WBMO5 and the Global ANN protein model WBP18.

Commodity	Origin	N, test	Range	Bias	*SEP*	*RPD*
WBMO5: European moisture ANN model						
6-row barley	NTEP, USA	126	7 – 21%	–0.16%	0.16%	14.1
WBP18: Global protein ANN model						
Wheat	CBH, Australia	1057	7 – 20%	0.00%	0.22%	9.7
Wheat	CGC, Canada	273	9 – 21%	–0.06%	0.24%	10.5
Wheat	Europe[a]	431	7 – 18%	0.07%	0.22%	7.6
Wheat	GIPSA, USA	480	7 – 21%	–0.04%	0.24%	11.7
Barley	CBH, Australia	489	7 – 17%	0.02%	0.30%	5.1
Barley	CGC, Canada	43	9 – 14%	0.09%	0.25%	4.7
Barley	Europe[a]	322	8 – 15%	–0.02%	0.26%	4.9
Barley	GIPSA, USA	36	8 – 17%	0.08%	0.37 %	5.5

[a]Predictions from Austria, Belgium, Denmark, France (Limagrain and GIEI), Germany (Raiffeisen Nord and Doemens), Sweden and UK combined.

Results and discussion

Ring test

Somewhat surprisingly, the average results determined by combustion tended to be slightly lower than the results for Kjeldahl. Also, the results from the European reference laboratories tended to be higher than those from Australia and North America. On the whole, however, the bias differences between the participating laboratories were small. The lowest bias value was 16.0 % protein (dm) and the highest 16.6%. The SD of the biases was 0.14%. It was, therefore, concluded that, apart from the harmonisation previously applied to the European protein values, no further adjustment was required.

Moisture

The results of the test performed by NTEP in the USA with American 6-row barley samples, using the European ANN-model WBMO5, are shown in Table 2. This accuracy is very good, as indicated by the low *SEP* and the high *RPD* values, reflecting the fact that the prediction curve is perfectly linear over the entire range. During the 1998 harvest in Denmark, linearity of the ANN–moisture models was demonstrated even at moisture levels above 25% moisture, while the PLS models failed at moisture levels over 18%.[2] The NTEP results also demonstrate the universal nature of the calibration, as the model was based entirely on European samples while the samples tested were all American. Another example of the broadness of the moisture calibration is reflected in the fact that i.a. triticale *(Triticosecale)* is well predicted without samples of triticale being present in the model.[2] Similar results with samples from other continents have confirmed that the European ANN moisture model is globally applicable; has a very broad commodity range; is linear even at very high moisture levels and is highly accurate.

Protein

The results of the predictions of protein in wheat and barley from various continents are also shown in Table 2. The prediction biases found with the various data sets are all close to zero. This observation indirectly confirms the small bias differences found in the intercontinental ring test between the participating reference laboratories.

For wheat, the *SEP* values for the various sample sets are small and highly consistent; the variation found in the RPD values is, thus, mostly caused by differences in range. It should be noted that all the North American wheat classes, including durum wheat, are well predicted with the global model.

The *SEP* values for barley are slightly higher than those for wheat. One explanation for this could be the fact that more than 20,000 wheat samples were available as compared with only 8,000 samples of barley, *cf*. Table 1. This is in agreement with the fact that there were very few barley samples from the USA in the model and that the samples from GIPSA were less accurately predicted than the other barley data sets. Canadian barley samples, on the other hand, were well predicted, perhaps because the growing conditions and varieties tested are more similar to the numerous (mostly North-) European samples. As with moisture, all the prediction curves were linear over the entire range, except for a couple of European wheat samples with protein levels below 8% (dm basis).

By comparing the present results for protein in European wheat and barley samples using the present global ANN calibration with similar predictions based on the previous European model (data not shown here), the accuracy for European samples apparently does not deteriorate when alien samples, such as the Australian ones, are introduced into the model.

The ANN model is currently being tested with samples from other continents, with results comparable to those presented here. It can, thus, be concluded that the ANN protein model is globally applicable; has a broad commodity range; is linear over the entire protein scale and its accuracy is satisfactory.

Conclusions

The practical experience with developing and using ANN calibration models can be summarised as follows:

ANN mathematics can handle extremely large data sets and any sign of saturation has yet to be observed.

It would appear that new data can, usually, be added to an ANN calibration without upsetting the accuracy of the existing model. In one case, the addition of a limited number of samples, representing just 1% of the samples in the previous model, were sufficient to correct a deficiency in the model.[2]

ANN mathematics can handle non-linear phenomena, which probably occur more often than we used to think.

ANN models, based on large data sets, are superior to PLS models both in terms of accuracy, broadness, stability and transferability.

Global ANN models are now available for protein in wheat and barley and for moisture in cereals, including wheat and barley. These models were used commercially in several European NIR transmittance networks in 1999.

The strategy followed to develop the present models can probably also be applied to other commodities and/or parameters.

The key to success for such future projects lies with the provision of large, consistent data sets which, again, calls for extended international co-operation.

Finally, it should be emphasised that non-linear mathematics in itself, of course, does not suffice to develop good models. The state of the optics, the data pre-processing, the size and diversity of the data set and the reliability of the reference values are, of course, all factors of equal importance.

Acknowledgement

The kind permission of the members of the participating networks allowing their data to be presented at NIR-99 is hereby gratefully acknowledged.

References

1. N.B. Büchmann, "NIR Networking—the ultimate control," in *Near Infrared Spectroscopy: The Future Waves*, Ed by A.M.C. Davies and P Williams. NIR Publications, Chichester, UK, pp. 479–483 (1996).
2. N.B. Büchmann, H. Josefsson and I.A. Cowe*, Accuracy, stability and transferability of the common European artificial neural network (ANN) calibrations for the determination of moisture and protein in cereals using the Danish Infratec 1221/1229 near infrared transmission (NIT) system*, to be published.
3. I. Sproul, Pesonal communication (1999).