Comparison of linear and non-linear near infrared calibration methods using large forage databases

Paolo Berzaghi,[a,b*] Peter C. Flinn,[c] Pierre Dardenne,[d] Martin Lagerholm,[e] John S. Shenk,[f] Mark O. Westerhaus[f] and Ian A. Cowe[e]

[a]*University of Padova, Agripolis, 35020 Legnaro, Italy*

[b]*University of Wisconsin, 1925 Linden Dr., 53706 Madison, WI, USA*

[c]*Agriculture Victoria, Pastoral and Veterinary Institute, Private Bag 105, Hamilton, Victoria 3300, Australia*

[d]*Centre de Recherches Agronomiques de Gembloux – CRAGx, 24 Chaussee de Namur, 5030 Gembloux, Belgium*

[e]*Foss Tecator AB, Box 70, SE-263 21 Höganäs, Sweden*

[f]*Infrasoft International, 109 Sellers Lane, 16870 Port Matilda, PA, USA*

Introduction

Forages represent about 50% of the diet fed to dairy cattle and information about their chemical composition is necessary to correctly balance nutrients in the diet. However, chemical and nutritional composition of forages is highly variable. Major sources of variation include botanical family (for example, legumes *vs* grasses), stage of maturity at harvest, method of conservation (for example, hay *vs* silage) and climatic conditions. As a result of these sources of variation, commercial forage testing labs have been using several different near infrared (NIR) calibrations to cover the analysis of all forages. Type and source of the sample is critical for the selection of the appropriate calibration equation and this information is often missing or incorrect. Forage NIR analysis would be simplified by using few or even only one NIR calibration for all types of forage. However, the large source of variation that the calibration data set must include may cause problems of non-linear relationships between spectral and chemical information resulting in lower accuracy of prediction.

Alternatives to multivariate calibration methods that can handle non-linear relationships are artificial neural network (ANN)[1] and local partial least squares (PLS) calibrations (LOCAL).[2] Although these methods are not new, they have only recently been introduced in practical applications and they were not tested with a large forage database. The aim of this study was to compare the performances of modified PLS (MPLS) calibration to ANN and LOCAL calibrations for the prediction of a large forage data set.

Near Infrared Spectroscopy: Proceedings of the 10th International Conference

Materials and methods

The study used historical forage data sets (25,977 samples) from Australia, Europe (Belgium, Germany, Italy and Sweden) and North America (Canada and USA). The data sets had already chemistry values relative to moisture (DM), crude protein (CP) and neutral detergent fibre (NDF) content that were obtained from different unharmonised laboratories. Samples spectra were collected during a time span of about ten years with ten different Foss NIRSystems instruments, which were either standardised or not standardised to one master instrument. The spectra were trimmed to a wavelength range between 1100 and 2498 nm.

Two data sets, one standardised (IVAL) and the other not standardised (SVAL) were used as independent validation sets but 10% of both sets were omitted from the validation sets and they were use for later expansion of the calibration database. The remaining samples were combined into one database (n = 21,696), which was split into 75% calibration (CALBASE) and 25% validation (VALBASE).

MPLS equations were developed using WinISI (Infrasoft International LLC, USA). Pre-defined spectral math treatments were first derivative, 4 data points skipping gap and smoothing with SNV-Detrend scatter correction. Local PLS calibrations were also developed under WinISI software. In this case, two settings were defined. The first was decided prior to the trial (LOCAL1), while the second (LOCAL2) was optimised for the prediction of CALBASE. There were also two methods for ANN (ANN1 and ANN2), both developed using Matlab (The Mathworks Inc., USA).

The chemical components in the three validation data sets were predicted with each model derived from CALBASE using the calibration database before and after it was enhanced with 10% of the samples from IVAL and SVAL data sets. Calibration performances were evaluated using standard error of prediction (*SEP*), bias, *SEP* corrected for bias [*SEP*(*C*)], slope and R^2.

Results

Regardless of calibration method, prediction of VALBASE (data not shown) had smaller *SEP*(*C*) and bias values than for IVAL (Table 1) and SVAL (Table 2). This was not surprising as VALBASE was selected from the calibration database and it had a sample population similar to CALBASE, whereas IVAL and SVAL were completely independent validation sets. Part of the problem may be caused by differences in wet chemistry methods, as indicated, for example, by the large bias of DM in SVAL or NDF in IVAL.

None of the models developed before enhancements appeared to be consistently better for the two independent validation sets. However, LOCAL and ANN had lower *SEP* and *SEP*(*C*) than MPLS for all three variables evaluated in VALBASE. This is consistent with previous studies that found LOCAL[3] and ANN[4] were able to handle data sets with large sources of variation.

In most cases, LOCAL and ANN models, but not MPLS, showed considerable improvement in the prediction of IVAL (Table 1) and SVAL (Table 2) after the calibration database had been expanded with the 10% samples of IVAL and SVAL reserved for calibration expansion. The addition of only 439 samples from the two independent sets to the 16272 samples of VALBASE greatly reduced bias, *SEP* and *SEP*(*C*) of LOCAL and ANN of IVAL and SVAL. From a practical point of view, the expansion of a database to predict new forage products will require fewer samples and result in better accuracy using either LOCAL or ANN than using MPLS calibrations.

The effects of sample processing, instrument standardisation and differences in reference procedure were partially confounded in the validation sets, so it was not possible to determine which factors were most important.

Table 1. Prediction performances of the different calibration methods for the independent set from Italy (IVAL).

	Enhancement	*SEP*	*SEP*(*C*)	Bias	Slope	R^2
DM (*n* = 1885)						
MPLS	Before	1.34	1.33	0.2	1.18	0.79
LOCAL1	Before	1.54	1.44	0.56	1.16	0.74
LOCAL2	Before	1.53	1.43	0.55	1.14	0.74
ANN1	Before	1.38	1.36	0.26	1.09	0.77
ANN2	Before	1.33	1.32	0.23	1.08	0.78
MPLS	After	1.33	1.32	0.17	1.17	0.79
LOCAL1	After	1.12	1.12	0.02	1.06	0.84
LOCAL2	After	1.07	1.07	0.01	1.06	0.85
ANN1	After	1.34	1.34	0.08	1.2	0.79
ANN2	After	1.32	1.32	0.09	1.18	0.79
CP (*n* = 1846)						
MPLS	Before	1.82	1.33	–1.25	0.88	0.96
LOCAL1	Before	2.12	1.52	–1.48	0.87	0.95
LOCAL2	Before	1.91	1.44	–1.26	0.87	0.95
ANN1	Before	2.15	1.54	–1.5	0.85	0.96
ANN2	Before	2	1.41	–1.42	0.87	0.96
MPLS	After	1.74	1.31	–1.14	0.89	0.96
LOCAL1	After	1.26	1.15	–0.51	0.96	0.96
LOCAL2	After	1.14	1.1	–0.3	0.97	0.96
ANN1	After	1.19	1.04	–0.57	0.95	0.97
ANN2	After	1.06	0.99	–0.39	0.97	0.97
NDF (*n* = 1912)						
MPLS	Before	4.62	3.47	3.05	1.02	0.93
LOCAL1	Before	5.53	4.15	3.66	0.99	0.89
LOCAL2	Before	5.36	3.82	3.76	1	0.91
ANN1	Before	4.64	3.56	2.98	1.06	0.93
ANN2	Before	4.98	3.46	3.59	1.05	0.93
MPLS	After	4.2	3.44	2.4	1.04	0.93
LOCAL1	After	3.4	3.2	1.16	1.02	0.94
LOCAL2	After	3.15	2.96	1.08	1.01	0.95
ANN1	After	3.15	3.06	0.77	1.04	0.94
ANN2	After	3.01	2.93	0.71	1.05	0.95

Table 2. Prediction performances of the different calibration methods for the independent set from Sweden (SVAL).

	Enhancement	*SEP*	*SEP(C)*	Bias	Slope	R^2
DM (n = 1861)						
MPLS	Before	3.85	2.41	–3.00	–0.26	0.12
LOCAL1	Before	3.08	2.46	–1.86	–0.15	0.05
LOCAL2	Before	3.20	2.43	–2.08	–0.11	0.03
ANN1	Before	3.30	2.41	–2.26	–0.20	0.07
ANN2	Before	3.52	2.49	–2.48	–0.23	0.11
MPLS	After	2.87	2.35	–1.64	–0.28	0.12
LOCAL1	After	0.90	0.90	–0.08	0.81	0.53
LOCAL2	After	0.90	0.89	–0.09	0.80	0.54
ANN1	After	0.82	0.82	–0.07	0.91	0.59
ANN2	After	0.66	0.66	–0.06	0.98	0.73
CP (n = 1860)						
MPLS	Before	1.01	0.74	0.69	0.97	0.97
LOCAL1	Before	1.34	1.06	0.82	0.98	0.94
LOCAL2	Before	1.56	1.32	0.83	0.96	0.92
ANN1	Before	1.21	0.70	0.99	0.94	0.98
ANN2	Before	1.27	0.72	1.04	0.96	0.98
MPLS	After	0.85	0.74	0.43	0.97	0.97
LOCAL1	After	0.74	0.74	0.00	1.00	0.97
LOCAL2	After	0.72	0.72	–0.01	0.99	0.97
ANN1	After	0.71	0.69	0.12	0.98	0.98
ANN2	After	0.67	0.67	0.09	0.97	0.98
NDF (n = 1660)						
MPLS	Before	2.60	2.39	–1.02	1.06	0.92
LOCAL1	Before	4.46	3.98	–2.02	1.03	0.78
LOCAL2	Before	3.63	3.60	–0.47	1.06	0.82
ANN1	Before	2.90	2.48	–1.49	1.06	0.92
ANN2	Before	2.53	2.53	–0.16	1.07	0.92
MPLS	After	2.27	2.27	0.08	1.04	0.93
LOCAL1	After	2.24	2.23	–0.18	1.03	0.93
LOCAL2	After	2.17	2.16	–0.17	1.04	0.94
ANN1	After	2.20	2.20	–0.13	1.03	0.93

Conclusions

Compared with MPLS, LOCAL and ANN improved accuracy in the predictions of forage samples similar to those in the calibration data set. The accuracy in the prediction of complete independent data sets was unacceptable for all models but LOCAL and ANN were able to reduce *SEP*, bias and *SEP*(*C*) after updates using a small number of samples. LOCAL and ANN were able to manage large sources of variation adding the flexibility of rapid and inexpensive expansion to new forage data sets.

Further work on the development of large databases must address the problems of standardisation of instruments, harmonisation and standardisation of laboratory procedures and, even more importantly, the definition of criteria for the selection of samples used in the creation and updates of the database.

References

1. T. Næs, K. Kvaal, T. Isaksson and C. Miller, *J. Near Infrared Spectrosc.* **1,** 1 (1993).
2. J.S. Shenk, P. Berzaghi and M.O. Westerhaus, *J. Near Infrared Spectrosc.* **5,** 223 (1997).
3. P. Berzaghi, J.S. Shenk and M.O. Westerhaus, *J. Near Infrared Spectrosc.* **8,** 1 (2000).
4. N.B. Buchmann, in *Near Infrared Spectroscopy: The Future Waves*, Ed by A.M.C. Davies and P. Williams. NIR Publications, Chichester, UK, p. 479 (1996).