Comparison of Benchtop and Handheld Near-infrared Spectroscopy Devices to Determine Forage Nutritive Value

NC STATE UNIVERSITY
Crop and Soil Sciences Department

Miguel S. Castillo[1], Juan J. Acosta[2], and Gary Hodge[2]

[1]Forage & Grassland Program, Crop & Soil Sciences Dept. and [2]CAMCORE, North Carolina State University, Raleigh, NC, USA

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Introduction and Objectives

The first step in development of NIR-models is collection of spectral data. Limited work, however, has been reported that compares predictions of basic estimates of forage nutritive value when using different NIR devices on the same sample. The objectives were to: 1) Develop and evaluate NIR spectroscopy models using three NIR devices with contrasting specifications to predict forage nutritive value, and 2) Compare predictions among three NIR devices.

Materials and Methods

Database Description and NIR Devices

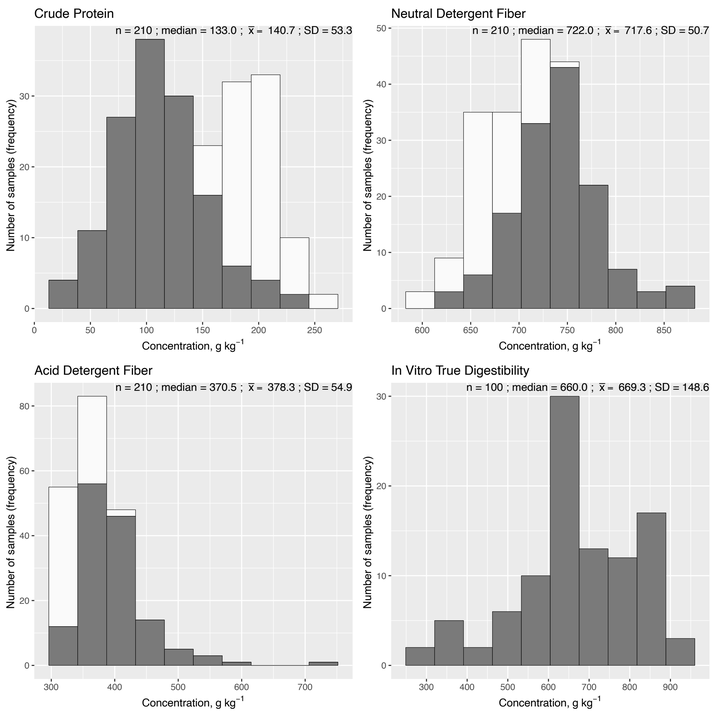

Fig. 1. Histograms and descriptive statistics of the databases. Filled bars correspond to switchgrass (*Panicum virgatum* L.) samples and white-filled bars to bermudagrass [*Cynodon dactylon* (L). Pers] samples.

Table 1. Near infrared devices

Device	ID	Type	Spectral Range (nm)	Wavelength interval (nm)	Number of Wavelengths
FOSS 6500 NIRSystems	FOSS	Benchtop	1100 – 2498	2	700
Thermo Scientific microPHAZIR	microPHAZIR	Handheld	1600 – 2400	8	100
Texas Instruments DLP NIRscan Nano EVM	Nano	Handheld	900 – 1700	5	160

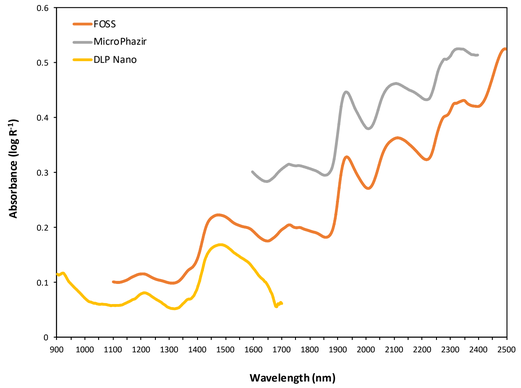

Fig. 2. Raw spectra measured by three near infrared spectroscopy devices. The plotted spectra correspond to the mean values of all scanned samples across instrument resolutions.

Chemometric Modeling

Model development was performed using a data analysis pipeline written in R environment. The pipeline has two separate phases: 1) transformations and outlier detection and 2) model training, cross-validation, and prediction of new observations. Fourteen scatter correction methods and spectral derivatives were applied to the spectral data. Local outlier factors (LOF) were used to filter-out atypical spectral data. Partial least squares regression (PLS) was implemented in R using the R-package 'pls' and model performance was evaluated using leave-one-out (LOO) cross-validation.

Results

Table 2. Fit statistics for models developed with 75% of the samples (training set) and validated on the remaining 25% samples (validation set) to determine crude protein (CP), neutral detergent fiber (NDF), acid detergent fiber (ADF), and in vitro true digestibility (IVTD) of switchgrass (*Panicum virgatum* L.) and bermudagrass [*Cynodon dactylon* (L.) Pers].

Equipment	Variable	Database†	Factors‡	R^2_c	SEC	R^2_cv	SECV	r^2	SEP
Foss	CP	MSC	16	.99	4.66	.99	5.87	.98	8.13
MicroPhazir	CP	NIR	7	.98	7.14	.98	7.81	.96	11.01
Nano	CP	NIR	12	.98	8.00	.96	10.11	.96	11.54
Foss	NDF	SNV	9	.90	15.79	.88	17.75	.87	19.08
MicroPhazir	NDF	MSC	8	.90	15.68	.87	18.48	.84	21.29
Nano	NDF	MSC_SG7	6	.91	15.15	.86	18.84	.81	23.84
Foss	ADF	SG7	6	.83	23.54	.79	25.98	.92	14.22
MicroPhazir	ADF	NIR	8	.84	22.57	.78	26.85	.86	19.96
Nano	ADF	SNV_SG7	6	.84	22.44	.76	27.57	.87	19.05
Foss	IVTD	SNV_SG7	6	.99	13.78	.98	19.31	.97	26.77
MicroPhazir	IVTD	DT	3	.97	26.68	.96	29.01	.96	30.68
Nano	IVTD	SNV	13	.99	13.00	.96	30.69	.90	49.89

† SNV: standard normal variate; MSC: multiplicative scatter correction; DT_SG7: Detrend plus Savitzky-Golay smoothed spectra using seven points; NIR:log(1/R)
‡ Number of loading factors (latent variables) in the partial least square regression models
R^2_c: coefficient of determination, calibration.
SEC: standard error of calibration (g kg^{-1})
R^2_cv: coefficient of determination, cross-validation
SECV: standard error of cross-validation (g kg^{-1})
r^2: coefficient of determination, prediction.
SEP: standard error of prediction (g kg^{-1})

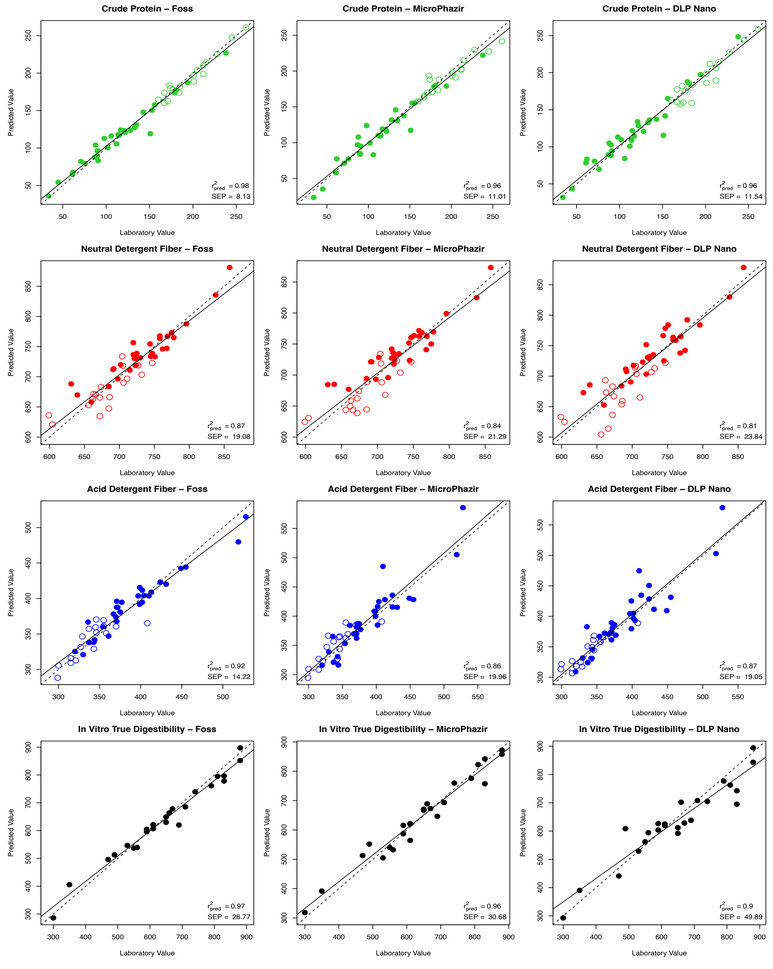

Fig. 3. Validation scatterplots of wet-chemistry values (ordinate) and near infrared (NIR) predictions (abscissa) for crude protein, neutral detergent fiber, acid detergent fiber, and in vitro true digestibility of bermudagrass and switchgrass samples. Closed circles correspond to switchgrass and open circles to bermudagrass samples. The dotted line in each figure represents a line with slope = 1 and the solid line represents the linear-regression line for the data.

Conclusions and Implications

- Different mathematical transformations for the same analyte were needed to optimized the NIR models for each device.
- Among devices, SEC, SECV, and SEP are comparable, and in some instances better, to the estimates of the NIRS Consortium level 2 equation release statistics for grass hay ('13GH50-2.eqa') and mixed hay ('16mh50-2.eqa').
- Consistently, the Foss models had the highest r^2-values; remarkably, the predictive power of the best models fitted for the other two handheld devices is very similar. These results warrant utilization and further applications of handheld devices.