Application of Near Infrared Reflectance Spectroscopy to Determine the Nutritional Composition of Soybean, Wheat and Maize

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Abstract

In this study, crop based NIRS calibration of proximate composition analysiswas, therefore, validated for soybean, wheat and maize, aiming at routine application of the model for screening materials at different stages of breeding. Results of the study showed that the coefficient of determination (R^2_V) ranged between 0.72 and 0.98, which indicated that there was a good relationship between measured and NIR predicated values, and standard error of prediction (SEP) was between 0.04 and 0.59, showing the robustness of NIRS calibrations. Except for crude fat in maize, which was less than 2, all relative percent deviation (RPD) values for other parameters ranged between 2.26 6.31, indicating higher performance of the equations for routine laboratory analysis. Therefore, these findings suggest that NIRS can be used in crop improvement programs and food formulation research to quickly and cheaply estimate nutritional composition of the tested crops.

Introduction

Knowing the nutritional compositionof food grains, such as wheat, maize and soybean is important, since nutrient content is a major quality criterea for selection of crop genotypes (Prasad *et al.*, 2016).

Conventionally,nutritional compositions, like protein and fat contents, of grain and other plant parts are analyzed by Kjeldhal and soxhlet methods, respectively, which are complex, labor intensive, chemical consuming and generally expensive. In contrast, NIRS (Near-infrared reflectance spectroscopy) is safe, non-destructive, efficient, and economical and environment 204.17 Tmpm[()-3(N)5(ea)-2(r)]TJETBT1 0Nron 249.0

or SH-containing compounds(Rosales b*et al.,* 2011).Even though NIRS method is simple, fast and less costly for routine laboratory analysis, the initial investment to develop a calibration model is high. Therefore, the common strategy would be to use global plant-based calibration developed By a Company with reliable NIRS database for various cereals, pulse and oil crops and bakery products (Foss AN52, 2011.

The calibration models contain a mixture of data from ground and unground grain samples over a wide range of concentration, which could be used for the determination of six parameters (fat, moisture, protein, crude fiber, ash and starch). However, before directly using these calibration models, there is a need to validate and check their suitability and performance to predict biochemical constituents in our materials (Foss AN52, 2011). Therefore, the objective of this study was to evaluate and validate global plant-based calibration for the determination of nutritional composition of soybean, maize and wheat for routine use of NIRS in laboratory analysis.

Materials and Methods

Plant material and sample preparation

Grain samples of 20 - 50 genotypes of each commodity were collected from the active breeding programs at Melkassa, Ambo, Bako, Pawe, and Kulumsa Agricultural Research Centers (for maize, soybean and wheat, respectively) and used for the validation of NIRS calibrations. The samples were selected in a way that would cover the range of concentration of the analytic of interest 50 - 100 seeds of each crop were ground using cyclone mill with 1 mm sieve (1094 cyclotec, FOSS). A sub-sample of the flour obtained from each sample was analyzed with reference analysis methods and the remaining was used for NIRS analysis.

Near infrared reflectance spectroscopy analysis

Ground samples were scanned in duplicate by NIRS spectrophotometer (FOSS NIR System, spinning model) using small ring cups with Foss Plant-based feed ingredient calibrations based on spectra from 400 – 2500 mm. Then, the predicted values for ash (%), moisture (%), crude fat (%) and crude protein (%) were recorded for external validation.

Chemical analysis to obtain the reference values

All the chemical analyses were done using Association of official Analytical Chemist (AOAC 2000) methods. Determination of protein content was done using Kjeldhal method (%) N multiplied by 6.25). Moisture content was determined using oven drying method and total ash was determined using furnace at 550 ^{0}C. Crude fat content was determined using soxtec extraction system (Soxtec 8000, Foss).

Mathematical procedures for validation

Independent validation of NIRS calibration involves determination and evaluation of coefficient of determination of validation sets (R^2v), which is the fraction of variance of the reference values explained by the variance of NIRS determinations and standard error of prediction (SEP), which is standard deviation (SD) between NIRS and reference determinations for validation sets, and RPD (relative performance deviation). This is the ratio of SD of the reference determinations to SEP (Rosales *et al.*, 2011).

Accordingly, the SEP and R^2v were calculated for the validation set. In addition, the ratio of SD to SEP was determined, as the quality and robustness of a NIRS calibration can be judged by the SEP and SD to SEP ratio (RPD less than 2 indicates an unsuitable calibration, between 2 and 3 is satisfactory for screening purpose. In addition, above 3 is assumed suitable for routine laboratory analysis (Rosales*et al*., 2011).

Results and Discussion

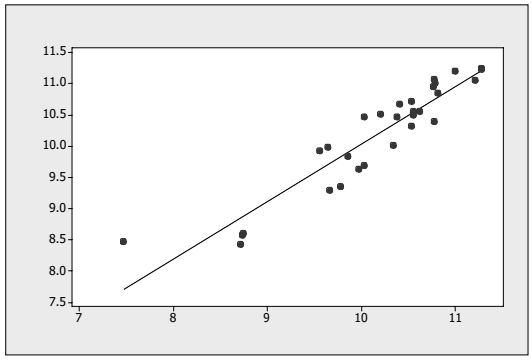
Maize

The result showed that R^2_V value of validation ranged between 0.72 – 0.98, which indicate that there is a good relationship between measured and NIRS predicated values, as R^2_V greater than 0.6 is acceptable. The SEP value was between 0.04 – 0.59, showing the robustness of NIRS equation for predicting proximate composition of maize. Except for crude fat, which was less than 2, all RPD values ranged between 2.26 – 6.31, indicating higher performance of the equations (as RPD value of 2.0 – 3.0 considered to be appropriate for screening and greater than 3 very satisfactory)for routine laboratoryanalysis in crop improvement programs (Rosales *et al*., 2011).

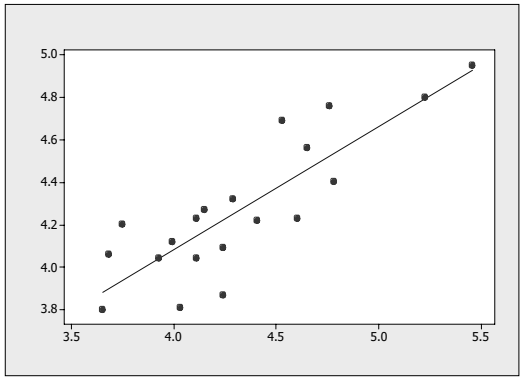
Table 2: Mean and range of reference values (%) and external validation statistics for CP, CF, MC and TA Contents in Maize grains.

Parameter	N	Range (%)	Mean (%)	SD	R^2_V	SEP	SD/SEP
Crude protein (CP)	30	7.8 - 11.28	10.17	0.85	0.87	0.31	2.70
Crude fat (CF)	20	3.65 - 5.46	3.74	0.48	0.72	0.26	1.82
Moisturecontent (MC)	40	9.53 - 12.98	10.96	0.97	0.98	0.15	6.31
Total ash (TA)	26	0.73 - 1.23	1.08	0.14	0.90	0.04	3.17

SD: standard deviation, R^2_V: coefficient of determination of validation sets, SEP: standard error of prediction, SD/SEP: SD to SEP ratio



(A)



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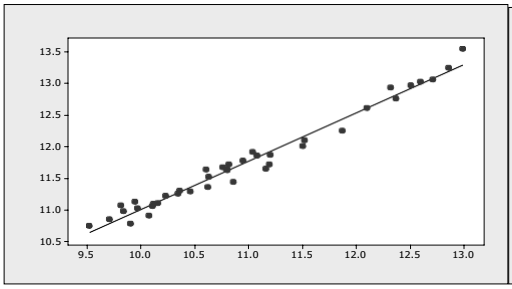
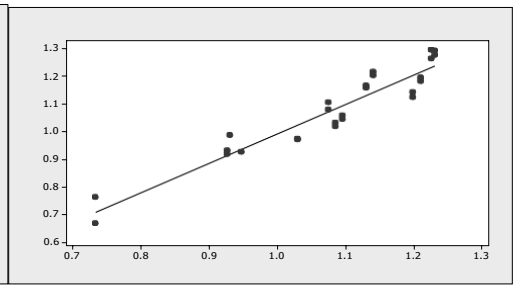




(c) **(d)**

Figuer 1 : Comparision of reference analysis values and NIR pridiction (a) crude protein, (b)crude fiber (c) moisture content and (d) total ash content in maize

Soybean

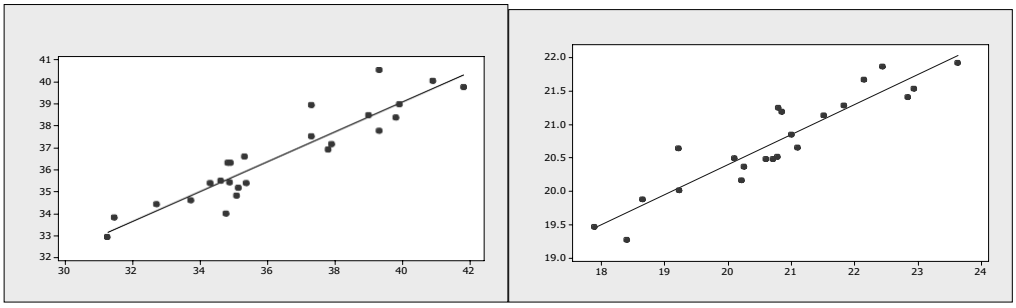
The R^2_V value of validation was 0.86 for both crude protein and oil contents of soybean, which indicates that there is a good relationship between measured and NIRS predicated values, (as $R^2_V > 0.6$ is considered acceptable). The SEP value for oil was 0.59 and for protein was 1.09, showing the robustness of NIRS equations for

predicting crude protein and oil contents of the crop. In addition, RPD values were 2.27 and 2.57 for protein and oil contents respectively, indicating higher performance of the equations (as RPD values of 2.0 – 3.0 are acceptable and > 3 Very satisfactory) for routine laboratoryanalysis in screening soybean genotypes based on oil and protein contents (Rosales *et al*., 2011).

Table 3: Range and mean reference values (%) and external validation statistics for crude protein and oil contents in soybean grain.

Parameter	N	Range (%)	Mean (%)	SD	R^2_V	SEP	SD/SEP
Crude protein	25	31.27 - 41.80	36.35	2.48	0.86	1.09	2.27
Oil (on dry matter basis)	22	17.89 - 23.63	20.78	1.51	0.86	0.59	2.57

SD: standard deviation, R^2_V: coefficient of determination of validation sets, SEP: standard error of prediction



(A) **(B)**

Figuer 2 : Comparision of reference analysis values and NIRS pridiction for: (a) crude protein and (b) oil content of soybean

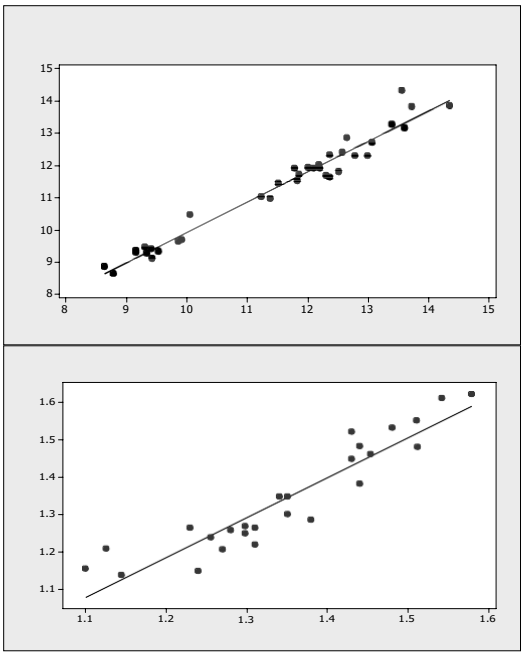
Wheat

R^2_V values of validation for wheat crude protein and ash content were 0.96 and 0.86, respectivelly.This result indicates that there is a good relationship between measured and NIRS predicated values, (where R^2_V values >0.6 are considered acceptable). The SEP for protein was 0.32 and for ash was 0.06, showing the robustness of NIRS equation. The RPD values were 5.05 and 2.26 for protein and ash content, respectively, indicating satisfactory performance of the equations (RPD values of 2.0 – 3.0 are acceptable and > 3 considered very satisfactory) for routine laboratory analysis in screening wheat lines for different end uses, such as pasta and bread.

Table 4: Range and mean reference values (%) and external validation statistics forcrude protein (CP) and total ash(TA) contents ofwheat grains

Parameter	N	Range	Mean	SD	R^2_V	SEP	SD/SEP
Crude protein (CP)	36	8.64 - 14.34	11.47	1.64	0.96	0.32	5.05
Total ash (TA)	27	1.10 - 1.58	1.35	0.13	0.86	0.06	2.26

SD: standard deviation, R^2_V: coefficient of determination of validation sets, SEP: standard error of prediction



(b)

Figuer 3 : Comparision of reference analysis values and NIR pridiction for : (a) crude protein and (b) total ash content of wheat grains

Conclusion

Performance of the calibration models in predicting validation sets was evaluated using mathematical procedures for each crop and parameter. Accordingly, the values of R^2_V, SEP and RPD fell in acceptable ranges and showed the existence of a close agreement between the measured and NIRS blind-predicted values of selected parameters of soybean, maize and wheat. Therefore, these findings suggest that NIRS can be used in crop improvement programs and food formulation research to quickly and cheaply estimate nutritional composition of the tested crops.

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