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# Use of near infrared reflectance spectroscopy (NIRS) for predicting soil fertility and historical management

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#### Abstract

This study tests the potential of near infrared reflectance spectroscopy (NIRS) for predicting soil fertility and management history from topsoil (0-10 cm depth) spectra. Soil fertility was assessed by measuring the growth of a test plant, and soil management history through inquiries with farmers. Moreover, NIRS predictive value was compared with that of a group of topsoil parameters: total carbon and nitrogen, nitrate, potential respiration and denitrification, and microbial biomass. Modelling used partial and modified partial least square regressions to ensure comparisons between predictions by NIRS ( $Q^2 = 0.78$  and  $R^2 = 0.89$  both;  $Q^2$  and  $R^2$  are cross-validation and calibration coefficient of determination, respectively), as were also the soil parameters ( $Q^2 = 0.79$ -0.92 and  $R^2 = 0.86$ -0.98). Soil fertility and management history were more accurately predicted by NIRS than by the set of soil parameters.

#### Keywords

Near infrared reflectance spectroscopy (NIRS); soil fertility; soil management; soil organic matter; microbial activity.

#### Introduction

The study of ecosystems and their components requires quantitative measurements of a diverse range of entities such as plants, animals, and the chemical components of soil or

water. The usefulness of near infrared reflectance spectroscopy (NIRS), as a non-destructive, quick and low-cost method to provide scientific expertise on a large scale, has been widely demonstrated up to now. The technique, originally adopted by agricultural and manufacturing industries, has progressively found applications in diverse scientific domains. From use on purely organic compounds, it evolved, for instance, towards soil and aquatic sediment analyses and proved in many cases very successful in these innovative uses. Several soil parameters have been investigated up to now, such as total carbon (C) and nitrogen (N) (Al-Abbas et al., 1972; Morra et al., 1991; Barthès et al., 2006), C and N mineralization (Palmborg and Nordgren, 1993; Chang et al., 2001; Ludwig et al., 2002; Schimann et al., 2007), microbial C and N (Reeves et al., 1999; Chang et al., 2001; Ludwig et al., 2002) or C and N distributions in particle size fractions (Barthès et al., 2008). However, although the use of NIRS has grown increasingly important for quantitative measurements, its application on more qualitative purposes has developed only very recently. There is a growing awareness that NIRS technology, providing wide and complex information, may be used successfully for evaluation of more integrative parameters of ecosystems functioning. Its use on multiple component materials, such as soil, requires multiple complex calibrations in order to extract the appropriate information from soil spectra. These complex procedures may unfortunately deter people from using the technique. It has nevertheless been used to examine phenomena as diverse as litter decomposition (Gillon et al., 1999), fodder digestibility (Park et al., 1998; Kitessa et al, 1999), wild animal feeding impact on vegetation (Stolter et al., 2006), agricultural yields (Terhoeven-Urselmans et al., 2008), soil management type (Reeves et al., 2001), and even past climate changes (Rosen et al., 2000).

These attempts to apply NIRS technology to new fields of research have generally yielded promising results and encourage hopes for further innovative applications. The present study follows this line of thought by testing two integrative parameters, soil fertility and soil management history. Evaluating these parameters requires labour intensive procedures, unlikely to be conducted over large areas. Being able to predict accurately these parameters with NIRS would thus allow large scale (agro-)ecosystem assessment and would therefore benefit both agronomical and ecological research.

The aim of the present work was: (1) to confirm the potential of NIRS to predict conventional soil parameters like total C and N, nitrate concentration, microbial biomass, basal respiration or denitrification potential; (2) to test the potential of NIRS to predict integrative parameters such as soil fertility and management history; and, in order to provide a benchmark of NIRS prediction relevance, (3) to compare the predictive value of NIRS with that of a group of

chemical and physiological variables of soil organic matter and microbial activity directly related to soil fertility and management history.

#### Materials and methods

#### Site

This study was conducted in Banh (14°04'N, 2°26'W), a village of the Lorum province, in the northern part of the Central Plateau of Burkina Faso. Banh is located in the southern Sahelian climatic zone, which is characterised by a 9-month dry season from September to May, and a 3-month rainy season lasting from June to August. Climatic data from 1971 to 2000 indicated a mean annual rainfall of 591 mm and a mean annual temperature of 28.7°C (Ouahigouya meteorological station, ~60 km south of Banh). The soil of the study area is described as a ferralic arenosol (FAO, 1998).

#### Plot characterization

Inquiries with farmers of the village of Banh were conducted in order to identify fields where livestock were or had been corralled. Fifteen farmer fields with regular goat and sheep overnight corralling were chosen. Inside these fields, each plot corralled in the past was also identified. Soil type was equivalent in all chosen plots. A farm survey was also done in order to check the homogeneity of all cultivation practices and to obtain a more complete management history for each plot. Plots influenced by the presence of surrounding trees or bushes, former burning of crop residues, or 'water drains' during the rainy season, were dismissed. Thus, 45 corralling plots were characterized in detail for the study, with time since corralling ranging from one to 11 years. In addition, 12 cultivated control plots without corralling were sampled, as well as 10 uncultivated control plots representing soil status before any cultivation and sampled at the border of the farmer field considered. A description of the yearly use of the fields can be found in Freschet et al. (2008).

#### Sampling

Samples were collected during the dry season. Within each plot, six samples were taken at random positions from the 0-10 cm soil layer. As cropping ridges of about 20 cm high were still present on cultivated plots during the sampling period, sampling was done on the ridges. These ridges were considered to represent the 0-10 cm layer of the cultivated soil. In uncultivated plots plant litter was removed before sampling. The samples originating from the same plot were pooled together, air-dried and sieved at 2 mm. Straw, gravels and faeces were

separated from the > 2 mm fraction and weighed. Gravels and straw, representing a very small proportion of the samples (respectively 0.39% and 0.04% of sample weight, in average), were not taken into account in this study. Faeces fragments > 2 mm were considered part of soil organic matter and returned to the soil samples. Samples were stored air dried at  $20^{\circ}$ C until further analyses.

#### Soil fertility

Soil fertility may be seen as the result of the combination of several parameters of soil organic matter, microbial activity and nutrient content. It is also quantifiable through the use of bioassays. The fertility of the soils under study was assessed using an experiment with a test plant (millet, *Pennisetum glaucum*) in small pots under greenhouse conditions. Each pot contained 150 g of soil and 10 seeds. Millet seeds were sorted before being sowed. Five replicate pots were established for each soil sample. Each pot received 25 ml of water daily during the 32 days of the experiment. After 32 days the entire plants (root and above-ground) were harvested and placed in a drying oven at 65°C. After 48 hours, the total dry biomass of each pot was weighed to determine the plant growth potential, expressed in grams. Millet growth potential was assumed to reflect soil fertility.

#### Soil management history

Soil management history may include very diverse information depending on the site, its use for agriculture, its climate and/or its socio-economical background. In the present context, soil is subject to 'mining agriculture'. Since all agricultural residues are harvested as forage and no inorganic inputs are returned to the soil, the only consistent inputs to the system are manure additions through livestock corralling. Due to a limited amount of livestock unevenly allocated between farmers, localized corralling in the fields and long intervals between corralling periods are managed by most farmers. The clearly identifiable position and time of the corralling within the fields provided an opportunity to study soil organic matter dynamics in the field. "Time elapsed since last corralling period" was therefore identified as the factor most fully representative of the agricultural history of a plot.

#### Soil organic carbon, total nitrogen and nitrate (NO<sub>3</sub>) content

Total soil was analysed for C and N by dry combustion on 0.2-mm ground sub-samples with a Fisons Na-2000 elemental analyser (Carlo Erba, Milano, Italy). Since there were no carbonates in these soils, soil total carbon ( $C_{tot}$ ) was considered as equal to soil organic carbon

( $C_{org}$ ) and expressed in mg C g<sup>-1</sup> soil. Total soil N ( $N_{tot}$ ) was expressed in mg N g<sup>-1</sup> soil. Soil nitrate content was determined colorimetrically in potassium chloride extracts (1 M) by flow injection analysis according to the method of Bremner (1965) and the result was expressed in  $\mu g$  N-NO<sub>3</sub><sup>-</sup> g<sup>-1</sup> soil.

#### Basal respiration and microbial biomass

Soil sub-samples (30 g of 2-mm sieved dry soil) were incubated at 100% of their waterholding capacities (80 µl of water per g of dry soil) in closed flasks (120 ml), maintained in the dark at 28°C during 7 days. During the incubation period, the carbon dioxide (CO<sub>2</sub>) respired in the flasks was analysed using direct injection into a micro gas chromatograph. After each CO<sub>2</sub> determination, the headspaces were flushed with fresh air. After 7 days of incubation, soil sub-samples were used for determination of microbial biomass. Potential basal respiration, expressed in µg CO<sub>2</sub>-C g<sup>-1</sup> soil d<sup>-1</sup>, was calculated when microbial respiration was stabilized, i.e. during the 3 last days of incubation. Microbial biomass N was determined by the fumigation-extraction method (Amato and Ladd, 1988) by measuring ninhydrin-reactive N compounds extracted from soils after 10 days of fumigation. Microbial biomass C (C<sub>mic</sub>) was estimated from the gain in ninhydrin-reactive N after fumigation per g of dry soil, multiplied by 21 (Amato and Ladd, 1988) and expressed in µg C g<sup>-1</sup> soil.

#### Denitrification potential

Denitrification potential was determined by measuring nitrous oxide (N<sub>2</sub>O) concentration in closed flasks after 48 hours of soil incubation at 28°C in the dark. Ten grams of 2-mm sieved dry soil sample were placed in a 60 ml flask with chloramphenicol (2.5 g per g of dry soil) and humidified at 100% of their water-holding capacity (80  $\mu$ l of water per g of dry soil). After 30 min to avoid priming effect, the air of the flask was replaced by a 90% helium, 10% acetylene gas mixture to ensure anaerobic conditions and inhibit N<sub>2</sub>O-reductase (Lensi et al., 1995). Five millilitres of a solution containing glucose (1 mg C-glucose per g of dry soil), glutamic acid (1 mg C-glutamic acid per g of dry soil) and sodium nitrate (100  $\mu$ g N-NO<sub>3</sub> per g of dry soil) were added to the soil. Air sample of each flask was measured by gas chromatograph. Denitrification potential was expressed in  $\mu$ g N<sub>2</sub>O-N g<sup>-1</sup> soil d<sup>-1</sup>.

#### NIRS analyses

Reflectance of the soil samples was measured between 1100 and 2500 nm at 2 nm intervals with a Foss NIRSystems 5000 spectrometer (Silver Spring, MD, USA), on two 5-g

subsamples per sample (2-mm sieved, oven-dried at 40°C). Each spectrum, averaged from 32 scans, was recorded as absorbance (log [1/reflectance]). Data analyses were conducted using the WinISI III-v.1.61 software (Infrasoft International, LCC, State College, PA, USA). Several mathematical pre-treatments were evaluated for spectrum pre-processing, in order to reduce baseline variations, enhance spectral features, reduce particle size effect and/or remove linear or curvilinear trends (Geladi et al., 1985; Barnes et al., 1989; Reeves et al., 2002): first or second derivatives with 4- or 5-point gap and smoothing (denoted 14, 15, 24 and 25, respectively), standard normal variate transform (SNV), detrending (D), and/or standard multiplicative scatter correction (MSC). A principal component analysis was carried out on spectral data for calculating the Mahalanobis distance H, and samples with H > 3 were considered spectral outliers and eliminated from further investigations (Mark and Tunnell, 1985). Calibration models deriving reference values from absorbance spectra were built using modified partial least square regression (mPLS): the mPLS regression reduces the spectral data to a few orthogonal combinations (or factors) of absorbance that account for most spectral information and relate to reference values, cross validation being recommended to estimate the optimal number of factors in order to avoid overfitting (Shenk and Westerhaus, 1991a, 1991b). Cross validation was performed by dividing the sample set into six subsets, five being used for developing the model and one for prediction, the procedure being performed six times to use all samples for both model development and prediction. The residuals of the six predictions were pooled to calculate the standard error of cross validation (SECV) and the corresponding coefficient of determination Q<sup>2</sup> (i.e. cross-validated coefficient of determination between predicted and measured values). Calibration outliers (i.e. with residual > 2.5 times SECV) were removed and another cross validation was performed, the procedure being carried out twice. The number of factors after which final SECV no longer decreased meaningfully determined the optimal number of factors of the model (Bjørsvik and Martens, 2001). The cross validation was appreciated by SECV, Q<sup>2</sup> and RPD (ratio of standard deviation to SECV; the meaning of the abbreviation varies with authors). Then, all remaining samples (i.e. outliers being removed) were used to calculate the final calibration model, which was evaluated by its standard error of calibration (SEC) and corresponding R<sup>2</sup> (coefficient of determination).

The main indicators used in this study to judge of the goodness of the results were: (1)  $Q^2$ , which is a measure of the goodness of fit of the cross validation, before the elimination of calibration outliers; (2)  $R^2$ , which is the coefficient of determination of the calibration model, once calibration outliers have been eliminated – both  $Q^2$  and  $R^2$  represent the predictive

quality of the model – and (3) RPD, which represents the predictive quality of the model through the standardization of the prediction error (SECV) against the variability of reference data.

#### Statistical analyses

To compare the capacity of NIR spectra vs. soil organic and biological variables to predict plant growth potential and time since corralling, partial least square (PLS) regressions (see Carrascal et al., 2008, for an insight into the test and its applications) and mPLS regressions were applied on both data sets (NIR absorbances vs. six soil variables). The mPLS regressions were processed with WinISI III-v.1.61 software (see sub-chapter on NIRS analyses) and PLS regressions were performed using the XLSTAT 2008 software (Addinsoft<sup>TM</sup>).

#### Results

The effect of corralling on soil properties was analyzed in Freschet et al. (2008). In short, soil organic matter, microbial activities and plant growth decreased exponentially with an increase in time since corralling, with duration and magnitude of the effect depending on the initial input of organic matter.

#### NIRS prediction of soil properties (Table 1)

The proportion of spectral outliers depended on the mathematical pre-treatment and represented 3% of the sample set in general (except in the absence of pre-treatment: 4.5%). The proportion of calibration outliers ranged from 10 to 20%, in general. The mathematical pre-treatment allowing the best calibration depended on the studied property (e.g. no pre-treatment for  $C_{tot}$  and  $N_{tot}$ , SNVD14 for N-NO<sub>3</sub> and  $C_{mic}$ ).

According to the soil property, the best cross validation yielded Q<sup>2</sup> values that ranged from 0.79 to 0.92, SECV from 24 to 85% of the mean, and RPD from 2.2 to 3.4. Best cross validations were very accurate for C<sub>tot</sub> and N<sub>tot</sub> (Q<sup>2</sup> = 0.90-0.92, SECV = 24-26%, RPD = 3.1-3.4), accurate for N-NO<sub>3</sub>, C-CO<sub>2</sub> and C<sub>mic</sub> (Q<sup>2</sup> = 0.81-0.86, SECV = 25-41%, RPD = 2.3-2.6), and acceptable for N-N<sub>2</sub>O (Q<sup>2</sup> = 0.79, SECV = 85%, RPD = 2.2). After discarding calibration outliers, best calibrations always yielded R<sup>2</sup> ≥ 0.86 and SEC ≤ 35% of the mean, and even R<sup>2</sup> ≥ 0.93, except for C<sub>mic</sub>, and SEC ≤ 22%, except for N-N<sub>2</sub>O.

#### NIRS prediction of soil fertility and management history (Table 1)

Soil fertility was assessed by millet growth for all 67 samples, from which 3% in general were spectral outliers (but 4.5% in the absence of pre-treatment), and 8 to 23% calibration outliers depending on the pre-treatment. The best calibration was achieved with SNV14.

Time since corralling was studied for cultivated plots only, which represented 57 samples, including those without corralling in order to increase the size of the sample set. The 12 cultivated plots without corralling were considered as plots where corralling had occurred a long time ago and was not detectable anymore through soil analyses. To estimate the period after which corralling effect was not detectable anymore, several values of time since corralling were tested for cultivated plots without corralling. The value that maximized spectrum fitting to time since corralling over the population of 57 cultivated plots was considered to represent the average period after which corralling was not detectable anymore. This period was found to be 15 years. Cross validation and calibration were subsequently performed considering that cultivated plots without corralling had been corralled 15 years ago. The proportion of spectral outliers was 3.5% and that of calibration outliers ranged from 5 to 18%. The best calibrations were reasonably accurate ( $Q^2 = 0.78$ ,  $R^2 = 0.89$ , SECV = 35-41%, SEC = 25-29%, RPD = 2.1-2.2; Figures 1 and 2).

#### Prediction of soil fertility and management history using NIR spectra vs. soil properties

Cross validation and calibration of millet growth were similarly accurate when performing PLS regression using NIR spectra and soil properties ( $C_{tot}$ ,  $N_{tot}$ ,  $C_{mic}$ , etc.): 0.69 vs. 0.66 for Q<sup>2</sup> and 0.76 vs. 0.78 for R<sup>2</sup>, respectively (Figure 3). Performing mPLS regression yielded much more accurate cross validation and calibration using NIR spectra than using soil properties: 0.78 vs. 0.37 for Q<sup>2</sup> and 0.89 vs. 0.47 for R<sup>2</sup>, respectively (data not shown). As for NIRS variables and mPLS regression (see above), several values of time since corralling were tested for cultivated plots without corralling for NIRS and soil variables, using PLS regression. For both NIRS and soil variables, the period that yielded the best results when cross validating and calibrating against time since corralling was 10 years and thus used as such for cultivated plots without corralling. When performing PLS regression, time since corralling was much less accurately cross validated and less accurately calibrated using NIR spectra than using soil properties: 0.15 vs. 0.50 for Q<sup>2</sup> and 0.42 vs. 0.54 for R<sup>2</sup>, respectively (Figure 4). On the contrary, performing similar mPLS regression yielded much more accurate cross validation and calibration of time since corralling using NIR spectra than using soil

variables: 0.78 vs. 0.37 for Q<sup>2</sup> and 0.89 vs. 0.37 for R<sup>2</sup>, respectively (data not shown). On the whole, NIRS and mPLS clearly yielded the most accurate cross validation and calibration of millet growth potential and time since corralling.

#### **Discussion and conclusion**

#### NIRS predictive potential

All studied soil properties were accurately cross validated and calibrated using NIRS and mPLS, with Q<sup>2</sup> values ranging from 0.79 to 0.92. Accurate NIRS predictions of C<sub>tot</sub> and N<sub>tot</sub> have been extensively reported (e.g. Al-Abbas et al., 1972, and Morra et al., 1991), especially for soil sample sets having rather homogeneous texture, where Q<sup>2</sup>  $\ge$  0.90 has frequently been observed (Brunet et al., 2007), as in the present study. Accurate NIRS predictions of soil basal respiration (Palmborg and Nordgren, 1993; Chang et al., 2001; Terhoeven-Urselmans et al., 2008) and potential denitrification (Schimann et al., 2007) have also been reported, with 0.82  $\le$  Q<sup>2</sup>  $\le$  0.94 ( $\le$  0.87 in general) and 2.0  $\le$  RPD  $\le$  2.3, which is consistent with the results of the present study. By contrast, the present results regarding NIRS prediction of microbial biomass C were more accurate than most published ones, which often displayed Q<sup>2</sup>  $\approx$  0.6-0.7 (Chang et al., 2001; Ludwig et al., 2002; Coûteaux et al., 2003; Terhoeven-Urselmans et al., 2006, 2008). Previous NIRS predictions of soil NO<sub>3</sub> have reported Q<sup>2</sup> < 0.55 and often < 0.4 (Malley et al., 2004; Viscarra Rossel et al., 2006), which contrasts strongly with the present study, possibly because it involved a rather homogeneous sample set.

The present study demonstrated that, beyond allowing the characterization of "intrinsic" soil properties such as  $C_{tot}$  or even  $C_{mic}$ , NIR spectra include information that involves numerous factors, such as plant growth potential or land management. Crop yield prediction using NIRS has rarely been reported in the literature. Van Groenigen et al. (2003) failed to predict rice yield and total vegetal biomass using NIRS ( $R^2 < 0.1$ ), and argued that the small range of variability within the field they studied might be the limiting factor in predicting these parameters. By contrast, Terhoeven-Urselmans et al. (2008) achieved accurate predictions of winter cereal yields on a range of soils:  $Q^2 = 0.77-0.90$ , RPD = 2.1-2.4 (depending on sample preparation), which is in line with present results. Using topsoil NIR spectra for predicting land management, as was done satisfactorily in the present study ( $Q^2 = 0.78$ ,  $R^2 = 0.89$ ), has been mentioned by Reeves et al. (1999) but they obtained poor cross validations for tillage (plow tillage vs. no-till) and N fertilization rate ( $Q^2 \le 0.52$ ,  $R^2 \le 0.67$ ). For the same sample set, Reeves et al. (2001) obtained much better results in the mid-infrared range (i.e. 2500-

25,000 nm) for tillage ( $Q^2 = 0.73 - 0.86$ ;  $R^2 = 0.87$ ), but not for N fertilization rate ( $Q^2 = 0.55$ ,  $R^2 = 0.69$ ).

#### Relevance of the use of NIRS in ecosystem studies

The promising perspectives offered by NIRS predictions of land management variables led to further test the robustness of NIR spectra. This was done by comparing it to the information contained in selected variables measured by routine laboratory analyses. It seems clear from these analyses that information contained in NIR spectra could be more informative than the routinely measured variables. The six variables chosen to define the soils were undoubtedly very informative but far from comprehensive in depicting soil fertility or management history. The NIR spectra, without being exhaustive either, seemed nevertheless better in this regard, their predictive value being seemingly robust despite integrating a range of varied phenomena.

Considering these results, it may be argued that the PLS regression used on soil variables may have been less powerful than the whole mPLS procedure used on spectral data. Indeed, if both methods allowed outlier elimination through principal component analysis and distance calculation, only the latter involved noise reduction and optimisation of spectral data through mathematical pre-treatments (derivation, etc.). The PLS regression gave better predictions than the mPLS regression when using soil variables, but a slight bias might have been introduced, coming possibly from the lower efficiency of mPLS regression on small data sets. Nevertheless, these statistical tests could be considered the most appropriate tools for providing the fairest possible comparisons.

#### Perspectives in the use of infrared spectroscopy

The primary advantage of NIRS is to allow comprehensive sampling schemes and high levels of replication by greatly improving the cost effectiveness of analyses. Its main benefit, as underlined by Foley et al. (1998), may however rest on its use as a complementary tool to explore areas hardly reachable with conventional means. In the present study, the use of NIRS permits the analysis of spectral properties of soils, which are related to chemical or biological soil properties that may not have been revealed by conventional analyses, and which have an influence on the parameter to be predicted (here millet yield or soil use). Besides, it should be remembered that reductionist approaches, although crucial in the understanding of process determinants and mechanisms, are often guided by the impossibility of directly observing integrative parameters. For instance, the choice of soil variables that were the focus the initial

study of Freschet et al. (2008) was partly guided by the goal of obtaining an integrative picture of soil 'health', 'quality', or 'fertility'. This example, among many others, stresses the fact that the overall aim of many studies rests in the understanding of how the different parts of a system are connected to work as a whole. In this respect, NIRS may be a powerful integrative tool in many agronomical or ecological studies. Exciting perspectives are still wide open for new ideas and concepts, hopefully facilitating a future large-scale use of NIRS in ecosystem studies.

The benefit of using of infrared spectroscopy in ecosystem studies can be further increased by combining it with geographic information system (GIS) techniques. Indeed, combining GIS and statistical methods with infrared spectroscopy assessments allows large scale mapping of ecosystem properties with good accuracy (Odlare et al., 2005; Wetterlind et al., 2008).

At present, great benefit would be derived from expanding the soil spectral library, notably by scanning previously characterized state and national soil archives (Brown et al., 2006). Using this data for NIRS calibration would allow extensive soil properties assessments, precision soil mapping and eventually soil properties monitoring through time. This approach should not be restrained to the soil compartment only. Its use is theoretically possible on components as diverse as soil microbes, plant litter or living plants. In the present context of rapid climatic and human-induced changes worldwide (Millenium Ecosystem Assessment, 2005), the potential of infrared spectroscopy to monitor changes in soil and plant properties through time and on large scales is of particular interest and needs to be thoroughly considered.

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- **Table 1.** Best results (depending on mathematical pre-treatment) for cross validation and calibration of soil total C ( $C_{tot}$ ) and N ( $N_{tot}$ ), potential respiration (C-CO<sub>2</sub>) and denitrification (N-N<sub>2</sub>O), nitrate-N (N-NO<sub>3</sub>), microbial biomass C ( $C_{mic}$ ), vegetal growth potential of millet, and time since corralling, using NIRS, outliers removed.

					Cr	Cross validation			Calibration		
Variable	Pre-	Ν	Mean	SD	SEC	SECV		RPD	SEC		R²
(unit)	treatment				(absol. value)	(%)	_		(absol. value)	(%)	
C <sub>tot</sub> (mg g <sup>-1</sup> soil)	none	52	7.05	5.78	1.68	24	0.92	3.4	1.28	18	0.95
$N_{tot}$ (mg g <sup>-1</sup> soil)	none	55	0.68	0.54	0.18	26	0.90	3.1	0.14	21	0.93
$N-NO_3$ (µg g <sup>-1</sup> soil)	SNVD14	56	32.08	30.25	13.07	41	0.81	2.3	6.50	20	0.95
C-CO <sub>2</sub> (µg g <sup>-1</sup> soil d <sup>-1</sup> )	MSC25	53	5.51	4.36	1.66	30	0.86	2.6	0.55	10	0.98
N-N <sub>2</sub> O (µg g <sup>-1</sup> soil d <sup>-1</sup> )	SNVD24	56	3.35	6.14	2.85	85	0.79	2.2	1.16	35	0.96
C <sub>mic</sub> (µg C g⁻¹ soil)	SNVD14	58	95.71	55.92	23.84	25	0.82	2.3	21.18	22	0.86
Vegetal growth (g)	SNV14	60	0.33	0.29	0.14	41	0.78	2.2	0.10	29	0.89
Time since corralling (yr)	SNVD24	46	7.04	5.25	2.49	35	0.78	2.1	1.75	25	0.89

N is the number of samples after outlier elimination.

SD is the standard deviation.

SECV and SEC are standard error of cross validation and of calibration, respectively; they are expressed as absolute values or as proportions of the mean.

Q<sup>2</sup> and R<sup>2</sup> are coefficients of determination for cross validation and calibration, respectively.

RPD is the ratio of standard deviation to SECV.

SNVD and SNV are standard normal variate transforms with and without detrend, MSC is multiplicative scatter correction, 14 is first derivatization with 4-point gap and smoothing, 24 and 25 are second derivatizations with 4- or 5-point gap and smoothing, respectively.

**Figure 1.** Comparison of plant growth potential as measured vs. as predicted by mPLS regression on NIR soil spectra, outliers removed.



**Figure 2.** Comparison of time since corralling as reported by farmers vs. as predicted by mPLS regression on NIR soil spectra, outliers removed.



**Figure 3.** Comparison of plant growth potential as measured vs. as predicted by PLS regression on NIR soil spectra (left) or on soil organic and biological variables (right), outliers removed.



**Figure 4.** Comparison of time since corralling as reported by farmers vs. as predicted by PLS regression on NIR soil spectra (left) or on soil organic and biological variables (right), outliers removed.

