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Predicting soil quality indices with near infrared analysis in a wildfire chronosequence

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Abstract

We investigated the power of near infrared (NIR) analysis for the quantitative assessment of soil quality in a wildfire chronosequence. The effect of wildfire disturbance and soil engineering activity of earthworms on soil organic matter quality was first assessed with principal component analysis of NIR spectra. Three soil quality indices were further calculated using an adaptation of the method proposed by Velasquez et al. [Velasquez, E., Lavelle, P., Andrade, M. GISQ, a multifunctional indicator of soil quality. *Soil Biol Biochem* 2007; 39: 3066–3080.], each one addressing an ecosystem service provided by soils: organic matter storage, nutrient supply and biological activity. Partial least squares regression models were developed to test the predicting ability of NIR analysis for these soil quality indices. All models reached coefficients of determination above 0.90 and ratios of performance to deviation above 2.8. This finding provides new opportunities for the monitoring of soil quality, using NIR scanning of soil samples.

Key words: NIRS; Soil quality; Soil health; Soil monitoring; GISQ; Soil biogenic structures

1. Introduction

Since the call of Haberern (1992) for a soil health index, several soil quality indices have been proposed (e.g. Breure, 2004). To be practical for management, such indicators should incorporate relevant information on physical, chemical and biological condition of soils (e.g. Doran and Safley, 1997; Zornoza et al., 2007). They should preferably be designed to assess a specific soil function (Andrews et al., 2004), a soil ecosystem service (Velasquez et al., 2007) or a soil threat (Morvan et al., 2008) in order to avoid the subjectivity of the soil quality paradigm debated in soil research (e.g. Sojka and Upchurch, 1999). GISQ, a general indicator of soil quality based on the provision of soil ecosystem services (Velasquez et al., 2007) fulfils most of these critical requirements. But since many soil analyses are involved, its implementation at the landscape scale remains too expensive and time consuming.

Near infrared reflectance spectroscopy (NIRS) is a rapid analytical technique involving diffuse reflectance measurement in the near infrared (NIR) region (1000-2500 nm). NIR spectra depend on the number and type of chemical bonds in the analysed material (Foley et al., 1998). NIR analysis is now widely used to predict soil carbon and nitrogen content (e.g. Brunet et al., 2007; Cécillon and Brun, 2007; Stevens et al., 2008). Its efficiency to predict soil biological properties (Cécillon et al., 2008) and to discriminate soil biogenic structures (e.g. earthworm casts) from surrounding soil (Hedde et al., 2005) has also been demonstrated. Recent developments of NIRS in soil research have shown its potential for a global assessment of soil quality (Vågen et al., 2006; Shepherd and Walsh, 2007) by discriminating different land-use types and soil degradation categories (Velasquez et al., 2005; Cohen et al., 2006; Awiti et al., 2008). However, the predictive capacity of NIRS for specific soil quality indices has not been assessed. In addition, the impact of an ecological factor such as wildfire (Rundel, 1981) on soil quality has not been tested *in-situ* with NIRS.

The objectives of this study were to assess (i) the efficiency of NIRS to detect the effect of wildfire and soil engineering activity of earthworms on soil organic matter (SOM) quality; (ii) the potential of NIRS for predicting soil quality indices derived from GISQ.

2. Material and methods

Soil samples were collected in the Maures mountains (Var, France) during spring 2007 in 25 plots depicting a heterogeneous mosaic of Mediterranean forests ecosystems generated by various wildfire frequencies. All soils were classified as Cambisols (IUSS Working Group WRB, 2006). Research plots were grouped into three classes depending on the time (t) since last fire (3 years, 16 years, > 50 years), each one including plots from different locations in the Maures mountains. In each plot, we collected two composite samples. One was made of earthworm casts collected at the soil surface, and the other one was made of twenty topsoil (0-5 cm) subsamples. For each sample, analyses addressing three soil ecosystem services were performed, according to Velasquez et al. (2007). Organic matter storage was assessed with organic carbon, total and mineral nitrogen content; nutrient supply was evaluated with pH and exchangeable cations (Ca, Mg, K, Na, CEC) and biological activity was assessed through microbiological parameters (microbial carbon, two extracellular enzymes –FDA hydrolase, cellulase– potential denitrification and microbial carbon to organic carbon ratio). The results of these soil analyses and their basic statistics are summarized in Table 1.

Three subindicators (SI) of soil quality reflecting the provision of each soil ecosystem service assessed were computed using a modified version of the GISQ approach (Velasquez et al., 2007). Briefly, for each group of variables (organic matter, nutrient supply, biological activity) we performed a principal components analysis (PCA) and a discriminant analysis (DA) to check the ability of groups of variables to significantly discriminate the six sample classes (three wildfire disturbances for two soil categories). Each of the three SI for one sample q is the sum of the n reduced variables (v_1-v_n , with $n = 4$ for organic matter, $n = 6$ for nutrient supply and $n = 5$ for biological activity) multiplied by their respective weight in the determination of axes 1 and 2 (w_1-w_n) of the PCA:

$$SI_q = w_1v_1 + w_2v_2 + \dots + w_nv_n$$

The set of values of each SI measured with the initial formula are finally reduced to constrain their variations within the range 0.1–1.0 using an homothetic transformation. Higher SI values indicate more ecosystem services produced, thereby an improved soil quality (Velasquez et al., 2007). Since the focus of this paper was on predicting specific soil quality indices (SI) with NIRS, no attempt was made to calculate a final GISQ value for each sample. The effect of wildfire disturbance and soil category on each SI was further assessed by analyses of variance (ANOVA) followed by Tukey's honest significant difference (HSD) test.

Diffuse reflectance measurements (1000-2500 nm) were carried out for each sample using a Fourier-transform NIR spectrophotometer Antaris II (Thermo electron) at a resolution $\Delta\lambda = 0.5$ nm ($\Delta\lambda$ is the smallest difference in wavelengths that can be distinguished) resulting in 6224 absorbance values per spectrum. The discrimination efficiency of NIR analysis for the six sample classes was assessed with a PCA of NIR spectra, using first derivative as spectral preprocessing. The unconstrained ordination of samples obtained with PCA illustrates the power of NIR data for a blind discrimination of samples without any *a priori* assumption on sample classes. Predictive ability of NIR analysis for the three soil quality indices was assessed through partial least square regression (PLSR, Tenenhaus, 1998). One NIR-PLSR model was built for each SI. Spectral pretreatment for PLSR included second derivative of spectra with selection of most important wavelengths by the variable importance on the projection (VIP) method (Wold et al., 1993), as described in a previous study using the same data set (Cécillon et al., 2008). The VIP method computes a score for each wavelength corresponding to a measure of its importance in the NIR-PLSR model. Only influential wavelengths with a VIP score greater than 1 were kept in the model. A new PLSR was then performed with selected wavelengths. The prediction performance of each obtained PLSR model was assessed by a full-model leave-one-out cross-validation (X-Val). Statistical treatments were conducted using R software version 2.6.1 (R Development Core Team, 2007) with *ade4* package for PCA and DA (Chessel et al., 2004), *pls* package for PLSR (Mevik and Wehrens, 2007) and the VIP algorithm of Chong and Jun (2005) as implemented for R software by B.H. Mevik.

3. Results and discussion

3.1. Tracking changes in soil quality with PCA of NIR spectra

The first two factors explained respectively 54 % and 20 % of the total variance in the PCA of NIR spectra (Figure 1). Axis 1 of PCA discriminated samples according to wildfire disturbance with steadily increasing scores from recently burned plots ($t = 3$ years) to control plots ($t > 50$ years), with an important contribution of the 1000 nm to 1800 nm range of wavelengths (Table 2). This result supports previously published studies (e.g. Pietikäinen and Fritze, 1995) describing a strong effect of fire on NIR spectra of soil samples usually explained by a change in organic matter quality after thermal modification of pre-existing C forms or production of pyrolysis compounds in burned soils (e.g. Gonzales-Pérez et al., 2004). However, this thermal effect on organic matter quality could not be assigned directly to organic carbon compounds since absorption bands of such compounds can be found throughout the NIR region (e.g. Malley et al., 2004). Axis 2 of PCA distinguished topsoil samples from soil biogenic structures, although discrimination was rather absent in recently burned plots (Figure 1). This result confirms the findings of Hedde et al. (2005) who identified specific functional signatures in NIR spectra of soil biogenic structures reflecting the deep change in SOM quality associated with the casting activity of earthworms. The detailed analysis of the PCA loadings for axis 2 revealed an important contribution of five NIR intervals within the range 1850-2500 nm (Table 2). This spectral region which also contains absorption bands assigned to organic carbon compounds was associated to soil microbiological activity in a previous study using the same NIR spectra (Cécillon et al., 2008). Earthworm effect on soil quality could thus be linked to changes in SOM quality and soil microbial processes (e.g. potential denitrification and potential nitrification).

3.2. NIR-PLSR models to predict specific soil quality indices

DA of the three groups of variables (organic matter, nutrient supply and biological activity) significantly classified each sample category ($p < 0.001$). No variables were removed from each group in the construction of the three SI. Soil biogenic structures obtained stronger SI values than topsoil samples for each soil quality indices ($p < 0.001$, Figure 2) stressing the importance of earthworms as ecosystem services providers (Lavelle et al., 2006). Earthworm casts were also characterized by a greater range of SI scores than topsoils except for SI biological activity (Figure 2). Fire effect on soil quality indices was weaker (Figure 2) but performing ANOVA tests revealed some clear trends. A significant increase ($p < 0.001$) in “SI Organic matter” was observed from recently burned plots ($t = 3$ years) to less disturbed plots ($t = 16$ years and $t > 50$ years). This trend was true for both topsoil and casts samples, indicating a recovery of SOM content after a wildfire event during vegetation regrowth. A significant effect ($p < 0.01$) of wildfire on “SI Biological activity” was also observed with control plots ($t > 50$ years) obtaining higher values than disturbed plots ($t = 3$ years and $t = 16$ years). This result suggests a long-term (> 16 years) negative effect of wildfire disturbance on the living soil. No effect of wildfire on “SI Nutrient supply” could be detected by ANOVA tests. PLSR models for the three soil quality indices reached “reasonable” (Williams, 1993) X-Val statistics with cross-validated coefficients of determination (Q^2) above 0.90 and ratio of performance to deviation (RPD) above 2.8 (Figure 2). These results are the first attempt of quantitative prediction of specific soil quality indices with NIRS. They confirm previously published studies which emphasized the potential of NIR analysis for a global assessment of soil quality (e.g. Velasquez et al., 2005; Cohen et al., 2006; Vågen et al., 2006).

4. Summary and conclusion

This study demonstrates that NIR analysis can be used as a powerful and inexpensive substitute for soil quality assessments compared to the conventional analysis. PCA of NIR spectra enabled rapid tracking of changes in soil quality driven by a disturbance such as wildfire. Soil quality indices

derived from an adaptation of the GISQ method were accurately predicted by PLSR of NIR spectra. Both approaches stressed the role of earthworms as soil ecosystem engineers, which improve soil quality through providing ecosystem services such as an increase in nutrient cycling, biological activity and SOM content. Our findings could have strong implications regarding programs for soil quality monitoring. Future studies should test the success of this strategy for larger and more variable data sets including different soil types. The current development of soil spectral libraries and the implementation of new chemometric techniques in soil spectroscopy research could facilitate this task.

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Table 1: Laboratory methods of soil analyses and summary statistics of reference data (n = 49)*

Soil ecosystem service	Property	Mean	SD	Reference method
Organic matter	Organic carbon (g kg ⁻¹)	52.2	28.0	NF ISO 10694 (1995)
	Total nitrogen (g kg ⁻¹)	2.94	1.43	NF ISO 13878 (1998)
	N – NO ₃ (mg kg ⁻¹)	17.5	26.1	Krom (1980)
	N – NH ₄ (mg kg ⁻¹)	21.7	25.6	Krom (1980)
Nutrient supply	PH in H ₂ O	6.42	0.34	NF ISO 10390 (2005)
	CEC (cmol+ kg ⁻¹)	15.5	5.1	NF X 31-130 (1999)
	Ca exch. (cmol+ kg ⁻¹)	11.2	4.1	NF X 31-108 (2002)
	Mg exch. (cmol+ kg ⁻¹)	2.42	1.07	NF X 31-108 (2002)
	K exch. (cmol+ kg ⁻¹)	0.72	0.27	NF X 31-108 (2002)
	Na exch. (cmol+ kg ⁻¹)	0.14	0.06	NF X 31-108 (2002)
Biological activity	Potential denitrification (µg N g ⁻¹ dw h ⁻¹)	0.26	0.23	Yoshinari et al. (1977); Smith and Tiedje (1979); Tiedje et al. (1989)
	Microbial carbon (mg g ⁻¹)	1.50	0.65	Anderson and Domsch (1978); Beare et al. (1990)
	Microbial carbon to organic carbon ratio	0.030	0.007	
	Cellulase (U ₁ g ⁻¹ dw)	0.015	0.008	Deng and Tabatabai (1994)
	FDA hydrolase (U ₂ g ⁻¹ dw)	0.0013	0.0004	Adam and Duncan (2001)

Abbreviations:

n = number of samples used to calculate summary statistics, to perform PCA and DA

SD = standard deviation; FDA = fluorescein di-acetate; dw = dry weight equivalent;

U₁ = µmol of glucose released min⁻¹; U₂ = µmol of fluorescein released min⁻¹

exch. = exchangeable

*: in one of the 25 plots, no earthworm casts could be collected above-ground, hence a total of 49 samples

Table 2: Wavelength intervals with highest loadings for the first two axes in the principal component analysis of NIR spectra

PCA axes	Main spectral intervals (nm)
PC 1 (Wildfire disturbance)	1000-1200; 1223-1351; 1510-1620; 1726-1827
PC 2 (Soil category)	1857-1903; 1920-1994; 2017-2086; 2223-2294; 2402-2500

Abbreviation:

PC = principal component

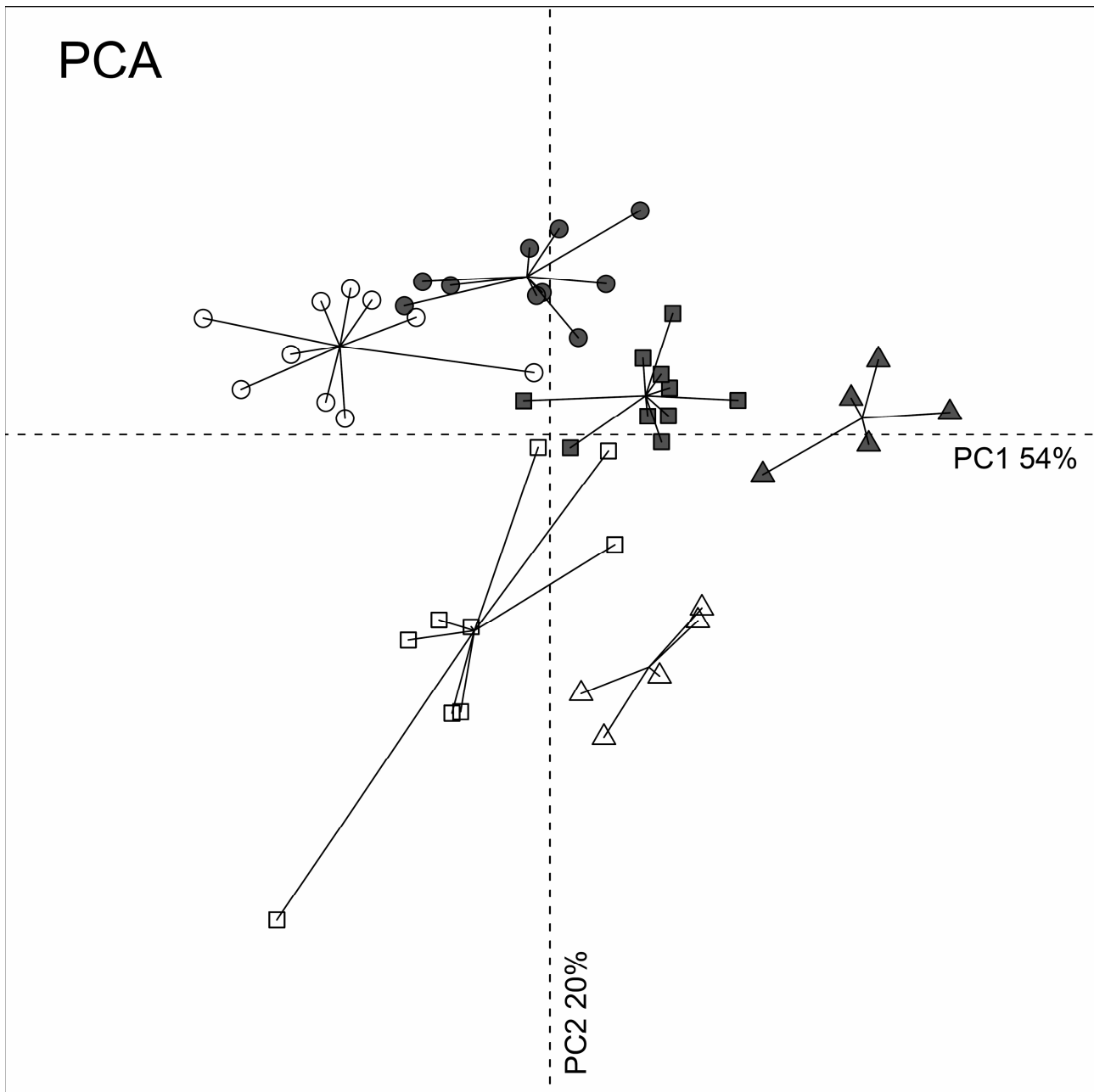


Figure 1: Principal component analysis of all samples calculated from the first derivative of the full NIR spectrum (1000-2500 nm). Grey symbols correspond to topsoil samples, white symbols are earthworm casts. Different symbols correspond to wildfire disturbance as described in the text (t = 3 years = circles; t = 16 years = squares; t > 50 years = triangles).

Abbreviation:

PC = principal component

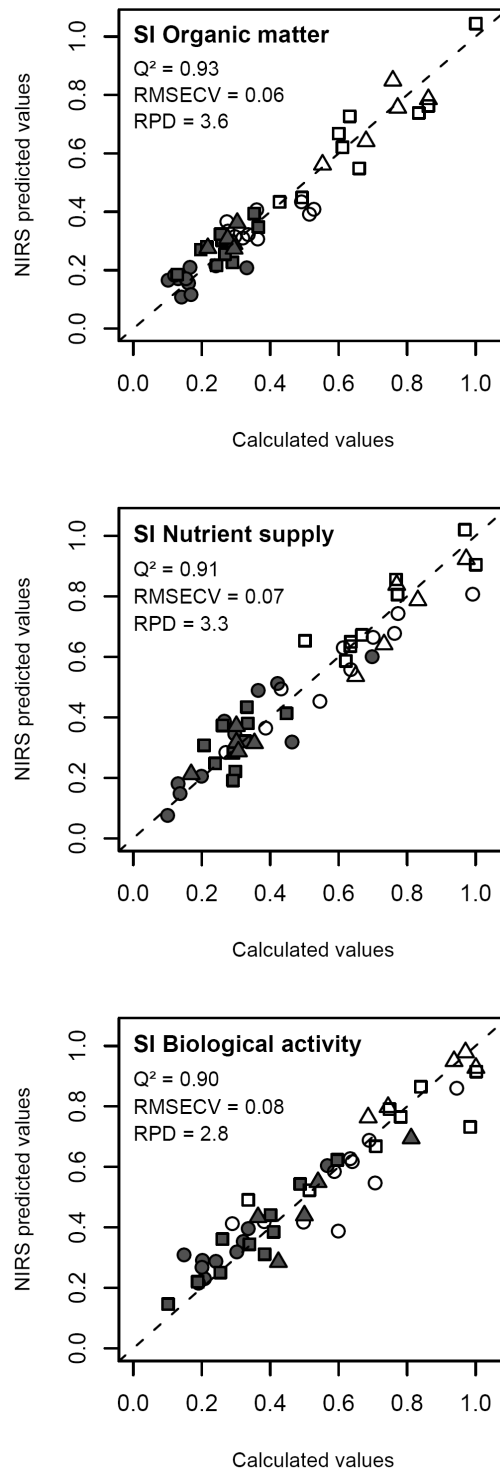


Figure 2: Scatter plots of NIRS predicted vs. calculated values for soil quality indices and X-Val results of PLSR models. The dashed lines indicate 1:1. The meaning of symbols is detailed in figure 1.

Abbreviations:

Q^2 = cross-validated R^2 ; $RMSECV$ = root mean squared error of cross-validation; RPD = ratio of performance-to-deviation (calculated as $RPD = SD\ RMSECV^{-1}$)