



Near infrared spectroscopy to quantify the temperature reached in burned soils: Importance of calibration set variability

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ABSTRACT

Near infrared (NIR) spectroscopy is a potential technique for the quantification of the temperature reached (TR) in burned soils. Due to spatial variation, inaccurate predictions can result from calibrating a model with heat-sensitive compounds that are not present in the samples of the burned area. Therefore, we investigated how to develop robust models. The progressive augmentation of the model size successively enhanced the precision, while the increase of the calibration set's variability gradually improved the accuracy through decreases in bias. The increase in calibration set variability enhances the probability of calibration using only the most common heat-sensitive compounds, facilitating reliable predictions of TR regardless of the spatial variation. On the other hand, models calibrated with heated aliquots from a unique sample, even from a composite sample, should be totally avoided because, regardless of their apparent utility, they are prone to inaccurate predictions.

1. Introduction

Fire is an important process in several terrestrial ecosystems throughout the world. The immediate fire effects on soil properties are mainly related with the fire severity, where the TR in soil is a crucial parameter (Neary et al., 1999; Vieira et al., 2015). Despite its importance, soil heating or TR in soil is a parameter neither measured by post-fire assessment teams, such as the Burned Area Emergency Response (BAER), nor by researchers, mostly due to the lack of a standard, easy, cheap, rapid and accurate method (Fernández and Vega, 2016; Parsons et al., 2010). Some of the existing methods are subjective (Vega et al., 2013), complex and expensive (Merino et al., 2014, 2015; Neris et al., 2014; Santín et al., 2016; Verdes and Salgado, 2011), have moderate accuracy (Melquiades and Thomaz, 2016; Perez and Moreno, 1998), or need several indicators to derive wide classes or levels, such as the soil burn severity index (Jain et al., 2008; Morgan et al., 2014; Parsons et al., 2010). To fill this gap, Guerrero et al. (2007) proposed the use of near infrared (NIR) reflectance spectroscopy as a potential technique for the quantification of TR in burned soils. The approach suggested by Guerrero et al. (2007) is based on two basic premises: i) the NIR spectrum of a soil sample contains information about the organic matter (quantity and quality), clay (quantity and quality), minerals (such as carbonates and iron oxides) and water content (Nocita et al., 2015; Stenberg et al., 2010; Viscarra Rossel and Behrens, 2010; Viscarra Rossel et al., 2016); and ii) these components have different sensitivity to thermal shocks (DeBano et al., 1998; Knicker, 2007; Neary

et al., 1999; Raison, 1979; Santín et al., 2016). Consequently, each temperature causes a group of changes in soil properties, leaving a typical fingerprint in the NIR spectra (Guerrero et al., 2007; Lugassi et al., 2010, 2014). Therefore, in this approach, the NIR spectrum is used as an integrative measurement of soil properties, which can be modified by the temperature (i.e., heat-sensitive compounds). However, as in other empirical approaches using NIR, a model is needed to relate the TR with its fingerprint in the NIR spectrum. For the development of such a model, soil samples are heated at known temperatures, which are used as standards (i.e., as calibration set) to calibrate the model. Hence, once the model has been calibrated (using chemometrics), the TR can be efficiently measured in very large numbers of samples because the NIR spectrum of a soil sample is obtained in seconds, easily and without the need of chemical reagents (avoiding the generation of toxic wastes in laboratories). To obtain high resolution maps of TR, which can serve to locate prior intervention areas in burned sites, it is necessary to measure this parameter (TR) in hundreds or even thousands of soil samples (Parsons et al., 2010; Jain et al., 2012). Additionally, the TR can provide relevant information for a better description of fire effects at very fine scale and to enhance the understanding of fire ecology, such as for the in situ analysis of fire-mediated germination patterns (Keeley et al., 2008; Lentile et al., 2007; Pausas et al., 2003).

The assessment of TR using NIR in a wildfire-affected area implies the collection of burned samples in those target points where TR is needed (for instance, for mapping) but also the collection of unburned

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soil samples to calibrate the model (Guerrero et al., 2007). As a consequence of the short-scale natural variation of the soil properties, a sample located at an arbitrary position (regardless if burned or not) may present its particular composition of heat-sensitive compounds, and this composition can differ with respect to other samples located at different positions. Two issues are imposed by the presence of spatial variation, which, through its design, a suitable model should overcome. The first is the impossibility of constructing a model using samples with similar composition to those to be predicted (except for planned events, such as prescribed fires). This limitation may exert a negative effect on prediction accuracy because the model might be fitted with heat-sensitive compounds that might not be the same as those present in samples located in the wildfire-affected area. The second implication is that the wildfire will affect samples with different heat-sensitive compounds; therefore, the model should be able to properly predict samples with different spectral responses. For these reasons, we found it interesting to investigate how we can develop robust models able to overcome such problems linked to the natural short-scale spatial variation. The calibration set characteristics play an important role in model performance. If the calibration set is composed by several different samples, only common heat-sensitive compounds (i.e., common spectral changes) should be used to fit the model. Consequently, accurate predictions are expected in those samples where the common heat-sensitive compounds are present. Therefore, the higher the variability included, the larger the commonality of the predictors, and the wider the model applicability. Thus, we hypothesised that increasing the calibration set variability should result in a progressive improvement of the predictions accuracy. To test the hypothesis, different model types were constructed and were then used to predict TR.

2. Materials and methods

2.1. Sites

This study was performed using forest soil samples collected in three different sites located in Alicante province (Spain): Aitana, Maigmo and Pinoso. These sites were approximately 30 km apart from each other. The vegetation of these sites is composed of *Pinus halepensis* Mill., as the dominant species in the tree stratum, the understory vegetation being dominated by species such as *Quercus coccifera* L., *Rosmarinus officinalis* L., *Juniperus oxycedrus* L., *Stipa tenacissima* L. and *Brachypodium retusum* (Pers.) P. Beauv. The main characteristics of the three study sites are given in Table 1.

2.2. Sample collection

In each site, five microplots (1 m²) were randomly selected in a small area of approximately 2500 m². The minimum and maximum distance between microplots was 5 and 50 m, respectively. In each microplot, a topsoil sample (0–5 cm depth) of approximately three kilograms was collected. These microplot-scale soil samples (hereafter MPS) collected in Aitana site were identified as A1, A2, A3, A4 and A5.

Table 1
Main characteristics of sites and soils characteristics (0–5 cm depth).

Site ^a	UTM coordinates ^b	T ^c (°C)	P ^d (mm)	Sand, silt, clay (%)	SOC ± SD ^e (%)	pH	CaCO ₃ (%)
A	30SYH3080	13.8	706	33, 32, 35	7.31 ± 3.11	7.5	46.9
M	30SYH0664	18.2	302	57, 22, 21	3.60 ± 1.23	7.9	57.6
P	30SXH7749	15.8	277	31, 56, 13	4.47 ± 1.64	8.0	7.0

^a A: Aitana; M: Maigmo; P: Pinoso.

^b UTM coordinates – WGS84 (at 1 km² resolution).

^c T: mean annual temperature.

^d P mean annual precipitation.

^e SD: standard deviation of the five MPS.

Those MPS collected in Maigmo were identified as M1, M2, M3, M4 and M5. Similarly, the MPS collected in the Pinoso site were identified as P1, P2, P3, P4 and P5. In each site, an additional “composite sample” was obtained by bulking several subsamples collected at different points across the whole area; these composite samples were identified as Ac, Mc and Pc for Aitana, Maigmo and Pinoso, respectively.

2.3. Obtaining standards (laboratory-heated samples)

Once in the laboratory, the 18 samples (15 MPS + 3 composite samples) were air-dried for two weeks (at 25 °C) and sieved to < 2 mm. These 18 samples were the “sources of standards”. Twenty-four aliquots of approximately 10 g were obtained from each sample. These aliquots were heated in a muffle furnace at 24 different combinations of temperatures (70 °C, 100 °C, 200 °C, 300 °C, 400 °C, 500 °C, 600 °C and 700 °C) and exposure times (10, 20 and 40 min). In this way, a set of 24 heated aliquots was obtained from each MPS sample (also from each composite sample). A total of 432 heated aliquots (24 heating combinations per sample × 6 samples [5 MPS + 1 composite] × 3 sites) were obtained, which were used as standards for the models (see Section 2.6). Each aliquot was introduced in the pre-heated furnace as a 1-mm layer in order to guarantee homogeneous heating (Guerrero, 2010). During the heating, to register the exact TR, the temperature of the aliquot was monitored and recorded every 10 s using a thermocouple (Guerrero et al., 2007).

2.4. Obtaining the NIR spectra of the heated aliquots

Once cooled, the NIR spectra (12,000–3800 cm⁻¹) of the 432 heated aliquots were obtained using a FT-NIR diffuse reflectance spectrophotometer (MPA Bruker, Germany). Further details about the scanning can be found in Guerrero et al. (2007). The x-scale of the spectra was transformed to nanometres (834–2630 nm) and resampled to 1 nm. All the spectra were transformed to absorbance, and then were pre-processed with the first derivative (Savitzky–Golay, 25 points) and vector normalization (Standard Normal Variate). The absorbance spectra of the 432 heated aliquots can be found as Supplementary content. The OPUS spectroscopic software (OPUS version 6.5 software; BrukerOptik GmbH, Ettlingen, Germany) was used for spectral pre-processing.

2.5. Regression method

We have constructed different types of models relating the TR with the NIR spectra (see Section 2.6). In all cases, the aliquots heated in laboratory (see Section 2.3) were used as the “standards” to calibrate the models. All models were calibrated with partial least squares (PLS) as the multivariate regression method, using the OPUS spectroscopic software (OPUS version 6.5 software; BrukerOptik GmbH, Ettlingen, Germany). The leave-one-out cross-validation was used to decide the number of PLS vectors to be included in models on the basis of the root mean square error of cross-validation (RMSECV) in a scree plot.

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