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Soil spectroscopy with the use of chemometrics, machine learning and pre-processing techniques in soil diagnosis: Recent advances -A review

Issam Barra[a,*], Stephan M. Haefele[b], Ruben Sakrabani[c], Fassil Kebede[a]

[a.] *Center of Excellence in Soil and Fertilizer Research in Africa, Mohammed VI Polytechnic University, Benguerir, Morocco.*
[b.] *Department of Sustainable Agriculture Sciences, Rothamsted Research, Harpenden, UK.*
[c.] *School of Water, Energy and Environment, Cranfield University, UK.*

Corresponding author:

*I. Barra, Center of Excellence in Soil and Fertilizer Research in Africa, Mohammed VI Polytechnic University, Benguerir, Morocco, Email: Issam.barra@um6p.ma

ABSTRACT

Over the past two decades soil spectroscopy, particularly, in the infrared range, is becoming a powerful technique to simplify analysis relative to the traditional chemical methods. It is known as a rapid, cost-effective, quantitative and eco-friendly technique, which can provide hyperspectral data with narrow and numerous wavebands, both in the laboratory and in the field. In this context, the present article reviews the recent developments in mid and near infrared techniques coupled with chemometrics and machine learning tools in addition to the preprocessing transformations and variable selection strategies to diagnose soil physical and chemical properties. Both spectral techniques demonstrated a good ability to provide accurate predictions of specific properties. Moreover, the MIR spectroscopy outperformed NIR for the estimation of most indicators used for fertilizers recommendation. Herein, a detailed overview on the opportunities and challenges that soil spectroscopy offers as efficient diagnostic tool in soil science was provided.

Keywords: Soil diagnosis, infrared spectroscopy, chemometrics, machine learning, data preprocessing

1. Introduction

Quantitative and qualitative analyses of soil properties ensure acquiring proper knowledge and skills for managing soil fertility and productivity through development of adjusted fertilizer formulations and recommendations [1]. The conventional soil laboratory methods require the use of chemical reagents, which are often not eco-friendly, a whole range of sophisticated laboratory equipment, and, moreover, the protocols are time consuming and expensive. The use of infrared spectroscopy method has gained ground, not so much as a substitute of conventional soil measurements, but as an additional option providing efficient, rapid, robust and cheap methods for soil characterization.

Spectroscopic techniques are considered as physical methods of characterization that can be defined as the study of the interaction of electromagnetic waves in the ultraviolet, visible and infrared wavelengths with a the material under consideration [2]. Furthermore, these techniques have shown, when coupled with a multivariate data analysis, to be powerful tools for developing quantitative and classification models in many disciplines including food technology [3–5], petroleum engineering [6–11] and soil science [12–14] among many others. Nowadays, the application of chemometrics and machine learning techniques are among the most relevant tools to investigate the relationship between the chemical variables and the measured instrumental signals [15–17].

The present paper aims at bringing together the recent developments in the coupling of infrared spectroscopy in the medium and near ranges with chemometrics and machine learning including the preprocessing tools in soil spectroscopy to diagnose soil physical and chemical properties.

2. Spectroscopic fingerprints

Spectroscopic techniques operate at different ranges of electromagnetic radiation. Among the various techniques, in the field of soil analysis, spectroscopic application includes near infrared spectroscopy (NIR) between 4000 and 13000 cm^{-1}, visible-near infrared (Vis-NIR) spectroscopy (4000 to 28600 cm^{-1}), mid-infrared (MIR) analysis that comprises Fourier transform infrared spectroscopy (FTIR) and FTIR-ATR (attenuated total reflection) between (400 to 4000 cm^{-1}) and the Raman spectroscopy (500–1500 cm^{-1}). These non-destructive techniques are characterized by the ease of use since they only require minimal sample preparation, they do not require sample treatments with chemicals and reagents, and they do not generate chemical wastes (i.e., eco-friendly) [18,19]. In this review a comparison was caried out between two common spectroscopic techniques i.e. NIR/Vis NIR and MIR in order to assess their usefulness in coupling with machine learning techniques to facilitate the prediction of key soil properties.

3. Chemometrics/Machine learning tools

Chemometrics is a discipline of analytical chemistry that uses mathematical, statistical and computer applications to reveal the hidden information from chemical analyses in order to optimize processes and/or products [20]. Most of the techniques used in this discipline aim at reducing the dimension of the data at hand to highlight the relationships between the group of samples or between the spectra and selected variables. There are two main categories of chemometrics tools, namely the unsupervised (generally for data visualization) and the supervised methods (prediction).

3.1.Preprocessing tools

Several factors can affect the quality of the infrared spectra. These factors include the particle size of the samples [21] and the variations of the optical path [22]. This is why it is necessary to have a well-defined sample preparation and analysis protocol for each spectrometer [23]. With the purpose of reducing these interferences, thereby improving the predictive ability of the models, a pre-treatment is highly recommended to be applied to the raw data (Figure 1). The most commonly used treatments in the vibrational spectroscopy are smoothing (remove the high-frequency noise from samples) [24], mean centering (include an adjustable intercept in multivariate models) [25], derivatives (reduce the drift of the baseline and highlight some parts of the spectral information) [26–28], normalization (minimize errors presented due to the samples preparation step) [29], standard normal variate (eliminate the effect of uncontrolled variations, viz, instrument optical path) [30] and multiplicative scatter correction (mitigate problems arising from scattered light) [31,32].

Figure 1 here

Figure 1. Effect of different preprocessing tools on MIR spectra. A: raw spectra, B: first derivative, C: standard normal variate, D: second derivative.

3.2.Data visualization

The most used visualization method is the principal component analysis (PCA). A well-known exploratory method which is used to unveil the underlying structure of the data. This is achieved by reducing the dimension of the data, from a very high number (in the thousands of variables) into a few orthogonal synthetic variables called Principal Components (PCs) whose aim is to recover as much variation as possible in the data at hand[33]. The number of PCs can be chosen on the basis of the explained total variance.

3.3.Regression tools

The supervised techniques are generally multivariate calibration techniques. This encompasses tools that involve setting up a relationship between two matrices; the predictor variables **X** (fingerprints)**,** on the one hand, and the variables to be predict **Y (**quantitative response), on the other hand. The commonly applied multivariate calibration tools are the partial least squares regression (PLS) and orthogonal projections to latent structures [34,35], support vector machine regression (SVMR) [36], principal component regression (PCR) [35] and multiple linear regression [37].

4. Prediction of soil properties

As shown in Tables **1-3**, several studies were carried out using infrared fingerprinting (i.e., in the MIR and NIR/Vis-NIR infrared ranges) in combination with chemometric methods for rapid soil properties diagnosis.

4.1.Application of NIR and Vis-NIR spectroscopy

Relevant studies carried out for soil diagnostic using NIR/Vis-NIR spectroscopy techniques and chemometric/machine learning methods are listed in **Table 1** and discussed in the sections below.

4.1.1. Total and Organic carbon

Applications of NIR and Vis-NIR spectral techniques with the PLS algorithm were found to be efficient for evaluating the soil organic carbon (SOC) in soils [14,38–46], where the difference between all these studies are the type of soils, sample set representativeness**,** the number of soil samples, sample preparation, the preprocessing strategies and model validation methodologies.

Combining NIR and Vis-NIR spectral databases on the one hand and PLS regression on the other hand yielded results that showed a good agreement between measured and predicted values, indicating accurate SOC predictions. One study [47] evaluated the effect of dataset division methods on the model accuracy, i.e., 50 strategies for dividing the data into calibration and validation samples were tested with PLS-NIR as a calibration model to predict soil organic carbon. Several data preprocessing strategies were also compared. The results showed that the optimization of data set division combined with PLS could improve the model prediction. In addition, [48] studied the effect of the data size on the prediction of total carbon using three different algorithms, namely PCR, PLS and SVMR applied on the same Vis-NIR spectra. The results showed that the required minimum number of samples for calibration was 29 for PCR, 72 for SVMR and 130 for PLSR, which confirmed that the PCR was less sensitive to the sample size than PLS and SVMR. On the other hand, the three predictive models were better in terms of correlation and prediction errors RMSEP (Root Mean Squared Error of Prediction). [49] compared the performance of a miniaturized (mobile) and a conventional (bench-top) near infrared reflectance (NIR) spectrometer for characterizing soil carbon and nitrogen, concluding that the PLS model that was set up on the spectral data of the two instruments led to acceptable results. Furthermore, coupling Vis-NIR spectra with SVMR and using eight preprocessing methods led to an improvement of the prediction accuracy of soil organic carbon contents in soil samples [50]. The results indicated that the Savitzky-Golay (SG) derivative was the best preprocessing method to predict SOC from Vis-NIR-SVMR spectra. [51] investigated the prediction of SOC using PLS regression applied to Vis-NIR data belonging to three external soil spectral libraries at national, regional and field scales. The calibrated models based on the three datasets led to good results. Moreover, the field scale calibration using a local library led to more accurate predictions than calibrations using regional or national libraries, which nevertheless yielded good results when completed with some spiking samples (originating from the target fields). [51] explored the PLSR calibration method and its ability to predict SOC from Vis-NIR data. The results obtained confirmed that the proposed approach provided reliable estimates with a large coefficient of determination R^2 and small predictions errors. In [52] the performances of infield estimation of SOC using a portable Vis-NIR spectrometer and moist soils with a laboratory NIR instrument on dried soil samples were compared. The model on air-dry spectra outperformed the one obtained from fresh samples in terms of correlation between predicted and measured SOC values. The performance of a cheap, micro-electromechanical system NIR spectrometer coupled with PLS, SVM and Cubist tree model regressions for SOC and total carbon (TC) prediction was assessed by [53]. The results showed that the Cubist model predicted SOC and TC more accurately than PLSR and SVMR. [54] evaluated the precision of Vis–NIRS, LIBS (Laser Induced Breakdown Spectroscopy), and combined Vis–NIRS - LIBS spectral data for simulated in-situ soil profile total C, inorganic C and SOC measurement. The calibrated Vis-NIR and LIBS models predicted soil C satisfactorily although not very accurately. Even data fusion of Vis–NIRS-LIBS did not consistently increase the accuracy of soil C prediction.

4.1.2. *Soil pH*

The applicability of Vis-NIR, pXRF and sensor data fusion (Vis-NIR+PXRF) for rapid characterization of soil pH was investigated by [55] comparing linear PLS method with a non-linear SVMR method. The results showed that Vis-NIR, pXRF and their fusion can be used to predict soil pH through SVMR more accurately.

4.1.3. *Total Nitrogen*

NIR spectroscopy was evaluated as a commercial pre-sowing test to estimate soil N supply of irrigated rice in south-eastern Australia [56]. The performance of the calibrated model was satisfactory in terms of prediction error and correlation between the predicted and measured N uptake. A similar study was conducted [58] to predict the soil total nitrogen (TN) content using NIR spectroscopic techniques along with two algorithms (i.e., PLS and SVMR). The study revealed that the calibrated SVMR model outperformed the PLS algorithm in terms of correlation (calibration and validation) and error values (RMSEP). [57] studied the effect of soil moisture on TN prediction using the Vis/NIR-PLS method, after applying four spectral preprocessing approaches, namely Savitzky–Golay (SG) smoothing, SG smoothing followed by first derivative (FD), orthogonal signal correction (OSC) and generalized least squares weighting (GLSW). The results demonstrated that the strength of OSC and GLSW in eliminating the effects of moisture when estimating TN is superior. Consequently, the GLSW-PLSR approach was recommended for improved Vis/NIR estimation of TN content under different soil moisture conditions.

4.1.4. *Prediction of multiple soil properties*

Several research studies investigated the predictive ability of PLS applied to Vis-NIR spectra for the prediction of four soil properties, namely pH, free iron oxide, clay and $CaCO_3$ [58–60]. Accordingly, the prediction performances of the PLSR models were stable and globally accurate for the four selected soil properties. [59] compared Vis-NIR Spectrometers of different resolutions for the prediction of seven soil properties, namely extractable P, K, Ca, Mg, Al, SOC and CEC using PLS modeling. The two instruments (Veris and FieldSpec brands) yielded both good results, making it hard to conclude which one performed better. Other previous research [61] studied different modeling techniques, viz., PLS, MLR, RR (Regression Rules) and ANN (Artificial Neural Network) for predicting soil texture and the SOC. The study concluded that machine learning techniques such as RR and ANN combined with Vis-NIR spectral data can provide precise predictions. A similar study [62] tested the accuracy of combining PLS with NIR and Vis-NIR techniques as a soil multi-nutrient availability index. The coupling of PLS - Vis-NIR proved to be relevant since it accurately predicted plant available P, Ca, Mg and K. [63] confirmed that soil Vis-NIR spectroscopy can accurately estimate SOC, TN, pH and texture. [64] examined the effect of considering soil samples from different depths during calibration modelling on the accuracy using Vis-NIR spectroscopy for the prediction of SOC and SON. This study proved that collecting samples from various depths resulted in increasing the robustness of the developed models. A large, regional scale study was carried out to inspect the potential of the NIR spectroscopy coupled with modified partial least squares regression (mPLS) for measuring several mineralogical and physico-chemical properties of Brazilian soils [65]. The models gave good predictions of soil organic matter content, clay content and the amounts of kaolinite and gibbsite. In addition, Vis-NIR spectro-radiometers can be used to predict SOC and hot water-extractable C (HWE-C) contents accurately in a wide range of soil types and soil properties [66]. A comparison of four multivariate techniques (i.e., PCR, PLS, ANN and SVMR) was conducted for the rapid and accurate prediction of four soil properties, namely SOC, TN, total P (TP) and total K, using Vis-NIR spectral data [67]. It turned out that SVMR yielded the best predictions for SOC, TN, and TP, whereas ANN yielded the best predictions for TK. In [68] the applicability of Vis–NIR spectroscopic technique coupled with PLS for estimating eighteen different soil properties, namely coarse crumb, pH (H_2O), pH (KCl), cation exchange capacity, sand, silt, and clay contents, total nitrogen, soil organic carbon, total potassium, total phosphorus, soluble salts, free iron (Fe_2O_3), available phosphorus, aluminum saturation, exchangeable aluminum, bulk density (BD) and base saturation (BS) was tested. Good prediction values were found for pH, SOC, TN, Fe_2O_3, salt, and aluminum saturation whereas satisfactory results were found for sand, silt, clay, TP, TK, CEC, AP and Al_{ex} (**figure 2**). The study of a spectral data-mining system was designed to minimize or eliminate any subjective or random variation during model development for the prediction of SOC, $CaCO_3$ and CEC [69]. The effect of this algorithm was clear, and predictions of all parameters were successful with good correlations and low prediction errors. [70] examined the potential of Vis-NIR spectroscopy for the prediction and mapping of sand and clay fractions of soils in one irrigated field with clayey texture in Turkey. The results showed a good prediction performance for both sand and clay. [71] compared four different portable near infrared sensors with different sizes for the prediction of soil characteristics, viz., pH_{CaCl2}, CEC, TC, clay, sand, silt, K_{ex}, Ca_{ex}, Mg_{ex}, and Na_{ex}. The results showed that the four portable infrared sensors presented good prediction accuracy for clay, sand, total carbon, CEC, pH, exchangeable Mg and Ca, but were poor in predicting silt, exchangeable Na, and K. Moreover, the regression tree modeling (Cubist) outperformed PLSR. [12] provided an assessment of the performance of portable and miniature Vis-NIR spectrometer to predict soil properties (i.e., pH, SOC, TC, TN, CEC, Ca_{ex}, Mg_{ex}, Na_{ex}, K_{ex}, sand, silt and clay). The results showed that the small Vis-NIR spectrometer coupled with chemometrics tools was able to predict the proposed soil characteristics with acceptable correlations and errors. [72] studied the effect of soil particle size on the prediction of Na_{ex} by multivariate models (PLS and PCR) based on NIR spectroscopy. The results proved that particle sizes have an important effect on the multivariate predictions (particle sizes larger than 0.212 mm led to better predictive models). [73] applied the Vis-NIR spectroscopy combined with PLS, PCR and wavelet analysis for the prediction of SOC and TN in soil. The results suggested that wavelet analysis was a better method for capturing the absorption features of soil properties and determining SOC and TN content. [74] tested short wave Vis-NIR reflectance spectroscopy for the prediction of four soil properties, including SOC, Ca, K and Mg. The prediction models were successful for SOC estimation and less successful for the three remaining properties. [75] evaluated an in-field NIR instrument combined with the PLS algorithm to predict the contents of TN, SOC, K, S, P and the pH in soil. The obtained results in this work suggested that good predictions of TN, SOC, S, P, and pH were obtained using the portable NIR spectrometer. [76] developed a new MLR model for the proper estimation of soil potassium content. The calibrated model showed a high potential for soil potassium prediction. [77] studied the effect of six different soil-water contents on the Vis–NIR predictions of four soil properties. The results demonstrated that the contents of clay, silt, and sand were well predicted at different soil moisture levels, whereas the estimation of SOC was good at air-dry soil conditions. [78] evaluated the feasibility of Vis-NIR spectroscopy for rapid determination of the four Fe forms: total Fe (Fe_t), pyrophosphate-extractable Fe (Fe_p), dithionite-citrate-bicarbonate extractable Fe (Fe_d), and oxalate-extractable Fe (Fe_o). The results indicated that the nonlinear SVMR models performed better than PLSR models for the predictions of all Fe forms. Several other studies investigated the usefulness of NIR and Vis-NIR spectroscopy combined with chemometrics, viz., PLS and SVMR for the prediction of soil fertility indicators [79–85], and the calibrated models were in most cases of good quality .

Figure 2 here

Figure 2. PLSR models of each soil property using Vis-NIR spectroscopy. Reused with permission [68]

Table1. A summary of recent applications of NIR and Vis-NIR techniques in combination with multivariate calibrations for the prediction of soil properties. A: well predicted ($R^2 > 0.8$), B: acceptable prediction ($0.6 < R^2 < 0.8$), C: poor prediction ($R^2 < 0.6$))

IR technique	Multivariate calibration	Sample size	Predicted properties	References
Vis-NIR	PCR, PLS, SVMR	216	$TC^{A(PCR)}$	[48]
NIR	PLS	360	C^{A} and TN^{B}	[49]
Vis-NIR	PLS	291	SOC^{A}	[38]
Vis-NIR	PLS	148	$clay^{B}$, $CaCO_3{}^{A}$ and pH^{C}	[58]
NIR	PLS	400	SOC^{B}, TN^{B}	[86]
Vis-NIR	PLS	798	P^{C}, K^{C}, Ca^{B}, Mg^{B}, Al^{C}, SOC^{B}, CEC^{C}	[59]
Vis-NIR	PLS	201	SOC^{A}	[14]
Vis-NIR	PLS	95	$clay^{B}$, $sand^{C}$, $silt^{C}$, $CaCO_3{}^{B}$, free $iron^{B}$, CEC^{B}, organic $carbon^{C}$, pH^{B}	[60]
Vis-NIR	PLS, MLR, ANN, RF, RR	850	bulk density, $SOC^{B(ANN,RF,RR)}$, soil texture $^{B(ANN,RF,RR)}$	[61]
Vis-NIR	PLS, Cubist	11213	$SOC^{A(cubist)}$	[39]
NIR, Vis-NIR	PLS	36	TP^{A}, $clay^{A}$, pH^{B}, SOC^{B}, CEC^{B}, Na^{C}, K^{B}, Mg^{A}, Ca^{B}, Fe^{A},	[62]
Vis-NIR	SVMR	298	SOC^{B}	[50]

NIR	PLS	22	Mineralizable N^{A}	[56]
Vis-NIR	PLS	120	SOC^{A}	[51]
Vis-NIR	PLS	83	SOC^{B}, TN^{B}, pH^{C}, $Silt^{B}$	[63]
Vis-NIR	PLS	324	SOC^{A}, SON^{C}	[64]
Vis-NIR	PLS, SVMR	96	$SOC^{A(PLS)}$, pH^{C}, $TN^{A(PLS)}$, $CEC^{A(PLS)}$, $Sand^{A(PLS)}$, $Silt^{C}$, $Clay^{A(PLS)}$	[83]
Vis-NIR	PLS	255	pH^{C}, CEC^{C}, $Sand^{A}$, $Clay^{C}$, $Silt^{C}$, TC^{C}, TN^{C}, K^{C}, P^{C}, S^{C}, Fe^{C}, Cu^{B}, Mn^{C}, Zn^{C}	[84]
NIR	PLS	148	$Clay^{B}$, $Silt^{C}$, $Sand^{B}$, pH (H_2O and KCl)^{C}, TC^{B}, P^{C}, Mehlich III, Ca^{C}, Mg^{C}, K^{C}, Al^{C}, CEC^{B}, Mineralogical properties^{B}	[65]
Vis-NIR	PLS	48	SOC^{B}, HWE-C^{B}	[66]
Vis-NIR	PLS	138	pH^{B}	[55]
Vis-NIR	PCR, PLS, ANN, SVMR	148	$SOC^{A(SVMR)}$, $TN^{A(SVMR)}$, $TP^{B(SVMR)}$, $TK^{B(ANN)}$	[67]
Vis-NIR	PLS	146	$Sand^{B}$, $Silt^{B}$, $Clay^{C}$, pH(H_2O and KCl)^{A}, SOC^{B},	[68]

			TN^{B}, K^{B}, TP^{B}, CEC^{B}, $Fe_2O_3^{B}$, AP^{C}, Ex. Al^{C}, AS^{B}	
NIR	PLS, SVMR	90	$TN^{B(SVMR)}$	[87]
Vis-NIR	PLS	7120	SOC^{B}	[40]
Vis-NIR	PLS	514	TC^{B}	[41]
Vis-NIR	PLS, SVMR	149	$TC^{B(SVMR)}$	[88]
Vis-NIR	PLS	91	SOC^{A}, $CaCO_3^{A}$, CEC^{A}	[69]
Vis-NIR	MLR	28	K^{A}	[76]
Vis-NIR	PLS, SVMR	592	$Fe^{A(SVMR)}$	[78]
Vis-NIR	PLS, CCR	113	$SOC^{B(PLS)}$, Sand $^{B(PLS)}$, Silt $^{B(PLS)}$, Clay $^{B(CCR)}$	[85]
NIR	Mowing window PLS	91	SOC^{A}	[47]
NIR	PLS	431	SOC^{A}, TN^{A}, P^{B}, K^{B}	[79]
NIR	PLS	86	$Clay^{A}$, $Sand^{A}$	[70]
NIR	PLS, PCR	332	Exch. $Na^{B(PCR)}$	[72]
NIR	PLS	179	TC^{A}, TN^{A}	[81]
NIR	PLS	60	SOC^{A}, TN^{A}, $Nitrate^{A}$	[82]
NIR	PLS	384	TC^{A}, TN^{A}	[80]
NIR	PLS, SVM, Cubist tree model	151	$SOC^{B(Cubist)}$, TC $^{B(Cubist)}$	[53]

NIR vs LIBS	PLS, LASSO regression, MRCE	236	$TC^{B(PLS)}$, $SOC^{B(PLS)}$, $IC^{A(PLS)}$	[54]
Vis-NIR, NIR	PLS	392	$pH(CaCl_2)^B$, CEC^A, TC^A, $Clay^A$, $Sand^B$, $Silt^C$, Exch.(K^B, Ca^B, Mg^B, Na^B)	[71]
Vis-NIR	PLS	70	SOC^B, $Sand^A$, $Silt^A$, $Clay^A$	[77]
Vis-NIR	PLS	458	pH^B, SOC^A, TC^A, TN^A, CEC^A, Ca^B, Mg^B, Na^B, K^C, Sand, $Silt^B$, $Clay^A$	[12]
Vis-NIR	PLS	62	TN^B	[57]
Vis-NIR	PLS, PCR, wavelet analysis	60	$SOC^{A(WA)}$, $TN^{A(WA)}$	[73]
Vis-NIR	PLS	98	IC^B, TOC^B	[43]
Vis-NIR	PLS	20	SOC^A	[52]
Vis-NIR	PLS	168	SOC^B, Ca^C, K^B, Mg^C	[74]
Vis-NIR	PLS	194	SOC^B	[44]
Vis-NIR	PLS	173	SOC^A	[45]
Vis-NIR	PLS	12128	SOC^B	[46]
NIR	PLS	50	SOC^B	[42]
NIR	PLS	70	TN^B, SOC^B, K^B, S^A, P^B, pH^B,	[75]

4.2.The use of MIR spectroscopy

The coupling of MIR spectroscopy with chemometrics/machine learning modeling algorithms proved its capabilities to generate multivariate models that make it possible to rapidly perform a soil diagnosis. Relevant studies that were carried out using MIR spectroscopy and are summarized in **Table 2** and discussed in the sections below.

4.2.1. Soil organic carbon

[89] investigated data fusion strategies for laser-induced breakdown spectroscopy (LIBS) and attenuated total reflectance Fourier-transform mid-infrared spectroscopy (FTIR-ATR), as well as a combination of multivariate calibration methods (PLS, SVMR and ANN) for the prediction of soil organic carbon (SOC) content in soil samples. The findings from this work suggest that the use of LIBS and FTIR-ATR spectra in combination with multivariate calibration namely the ANN can be a fast and non-destructive approach to monitor SOC.

4.2.2. Phosphorus

[90] explored the application of MIR DRIFT in combination with chemometrics (PLS), for the prediction of one of the most important indicators of soil fertility and quality which is the P sorption property. The validation of the model to predict the P sorption index was satisfactory for most types of sorption.

4.2.3. Multi-prediction of more than one property

Recent work [12] proposed an effective approach based on portable MIR spectroscopy data modeled by machine learning techniques (Random Forest [RF] and PLSR) to predict TC, TN, CEC, clay, silt and Na_{ex} in 458 representative Australian soil samples. All models were proven to have a good performance with excellent results obtained by means of the RF algorithm. Early works [91] investigated the possibility of using diffuse reflectance infrared Fourier transform (DRIFT) spectroscopy to predict soil quality in the form of a soil quality index (SQI). To do this the infrared spectra were modeled using the PLS method for the prediction of the most important soil properties, namely pH both in water and KCl, $CaCO_3$, SOC, CEC, sand, silt and clay. The study demonstrated that DRIFT data could be calibrated to estimate a soil quality index by directly predicting measurable soil parameters. [92] tested a small portable prototype MIR spectrometer to collect soil spectra from two agricultural fields (predominantly organic and mineral soils). Those spectra were used for setting up PLS multivariate models for the prediction of pH, CEC, SOC, Ca, Mg, TN, TP, Fe, Cu, K, Na in Canadian soils. The results showed that in both organic and mineral soils, SOC, CEC, Ca and Mg were predicted with varying levels of accuracy. It was found that Fe in an organic soil field could be predicted with a moderate accuracy. [93] examined the ability of MIR to predict lime requirements (LR) of cultivated soils. The precision of the PLSR model was not sufficient to predict the spatial variability of LR. However, the authors suggested that MIR spectroscopy can be used to predict the averaged value of LR. [94] compared the coupling of mid-infrared spectroscopy with PLS and PLS-NN (Partial Least Squares combined with Neural Network) methods for the prediction of a wide range of chemical and physical soil properties. This study proved that the predictions using the novel PLS-NN approach appeared to be the most precise based on the coefficient of determination (R^2) and root-mean squared errors of prediction (RMSEP) values for total organic carbon (TOC) which were improved from $R^2 = 0.87$ and RMSEP = 0.7% by PLS, to an $R^2 = 0.94$ and RMSEP = 0.5% by PLS-NN. [95] The MIR spectroscopic technique combined with Random Forest was used to predict soil properties related to its fertility (pH, Mehlich-3 (i.e., Ca, K, Mg, Na, P, Al, B, Cu, Fe, Mn, Zn, S), P sorption, clay, sand, silt, TN and SOC). The prediction models from MIR spectra were good ($R^2 > 0.80$) for SOC and TN, pH and Mehlich-3 (Ca and Al); intermediate ($R^2 > 0.60$) for sand, silt, clay, P sorption index and extractable Mg and less satisfactory ($R^2 < 0.60$) for Mehlich-3 extractable K, Mn, Fe, Cu, B, Zn, P, S, and Na. The predictive performance of linear (PLS) and non-linear (SVM) multivariate regression models were evaluated by predicting four physico-chemical properties of soil (pH, sand, clay and TOC) using MIR spectral data [96]. The results showed that support vector machines outperformed PLS models for all soil properties tested. [97] compared the performance of the commercial OPUS Quant 2 software, which uses partial least squares regression (PLSR), with the PLS, ANN, and SVMR calibration algorithms. It turned out that, on the one hand, support vector machine regression slightly outperformed the other algorithms and resulted in better predictions and, on the other hand, the performance of SVMR and PLSR decreased when the sample size used for the calibration decreased. [98] used the diffuse reflectance spectroscopy (DRF), attenuated total reflectance spectroscopy (ATR) and Fourier transform infrared photoacoustic spectroscopy (PAS) coupled to the self-adaptive partial least squares model (SAM–PLS) to predict four soil properties and to explore their features in the Mid-Infrared range by the use of uninformative variable elimination (UVE) algorithm as a variable selection tool. The results showed that selected wavenumbers improved the accuracy of prediction for pH, SOC, TN and P contents. [99] proposed and developed simple methods for partitioning the African spectral library (Afsis) into subspaces from which local calibration models were developed and assessed against global models. The results proved that the global models were more accurate than the local ones. Furthermore, several researchers studied the performance of coupling MIR and PLS for the prediction of important soil properties [100–108]. The results generally led to successful predictions, **figure 3** shows as an example the result obtained by Waruru et al. [105].

Figure 3 here

Figure 3. Scatterplot for measured vs predicted values of selected soil properties for mixed depth data sets using MIR spectroscopy. LL: liquid limit, PL: plastic limit, PI: plasticity index, LS: linear shrinkage, COLE: coefficient of linear extensibility, VS: volumetric shrinkage, tClay: total clay content, tSa: total sand content, W: air-dried moisture content, CEC: cation exchange capacity. Reused with permission [105]

Table 2. A summary of the recent applications of MIR technique in combination with multivariate calibrations for the prediction of soil properties. A: well predicted ($R^2 > 0.8$), B: acceptable prediction ($0.6 < R^2 < 0.8$), C: poor prediction ($R^2 < 0.6$)

IR technique	Multivariate calibration	Sample size	Predicted properties	References
MIR	PLS, SVMR	933	pH$^{A(SVMR)}$, Clay$^{A(SVMR)}$, Sand$^{A(SVMR)}$, TOC$^{A(SVMR)}$	[96]
MIR	PLS, RF	458	TC$^{A(RF)}$, TN$^{B(PLS)}$, CEC$^{B(PLS)}$, Clay$^{B(PLS)}$, Silt$^{B(RF)}$, Na$^{B(RF)}$	[12]
MIR	PLS	225	P sorption^{B}	[90]
FTMIR-ATR	PLS	89	pH(H_2O, KCl)^{B}, $CaCO_3$^{B}, SOC^{B}, CEC^{B}, Sand^{B}, Silt^{B}, Clay^{B},	[91]
MIR	PLS	300	pH^{C}, CEC^{B}, SOC^{A}, Ca^{B}, Mg^{B}, TN^{C}, TP^{C}, Fe^{B}, Cu^{C}, K^{C}, Na^{B}	[92]
MIR	PLS	54211	SOC^{A}, CEC^{A}, pH^{B}, TN^{A}, Sand^{B}, Silt^{B}, Clay^{A}	[100]
MIR	PLS, ANN, SVMR	144	SOC$^{A(SVMR)}$, TN $^{B(SVMR)}$, Sand $^{B(ANN)}$, Silt $^{A(ANN)}$, Clay $^{B(ANN)}$	[97]
MIR	PLS, PLS-NN	964	pH (H_2O, $CaCl_2$)$^{B(PLS-NN)}$,Sand$^{B(PLS-NN)}$, Clay$^{B(PLS-NN)}$, Silt^{C}, Exch (Al,Ca, Mg, Na)$^{A(PLS-NN)}$, K^{C}, P-Sorption$^{A(PLS-NN)}$, TOC$^{A(PLS-NN)}$	[94]

MIR	PLS	255	Clay^{B}, Silt^{C}, Sand^{B}, Exch(Ca, Mg, Na, K)^{B}, CEC^{A}, SOC^{B},	[105]
MIR	PLS	291	pH^{B}, EC^{B}, TC^{A}, TN^{A},C/N^{C}, P^{C}, K^{C}, Clay^{B}, Silt^{C}, Sand^{C}	[104]
MIR	PLS	80000	TC^{A}, OC^{A}, CEC^{A}, $CaCO_3$^{A}, pH^{B}, Clay^{A}	[107]
MIR	RF	700	pH^{B}, Mehlich-3(Ca^{B}, K^{B}, Mg^{B}, Na^{C}, P^{C}, Al^{B}, B^{B}, Cu^{C}, Fe^{C}, Mn^{B}, Zn^{C}, S^{C}), P sorption^{B}, Clay^{B}, Sand^{B}, Silt^{B}, TN^{A}, SOC^{A}	[95]
FTMIR, LIBS	PLS	204	SOC^{B}	[89]
MIR	PLS	180	TOC^{A}, TN^{A}, TOC/TN^{A}, TP^{A}	[103]
MIR	PLS, ANN	20000	pH$^{A(ANN)}$, SOC$^{A(ANN)}$, IC$^{A(ANN)}$, TC$^{A(ANN)}$, TN$^{A(ANN)}$, clay$^{A(ANN)}$, silt$^{B(PLS)}$, sand$^{B(PLS)}$, M3 extractable (P)^{C}, K$^{B(PLS)}$, CEC$^{A(ANN)}$, S$^{A(ANN)}$	[108]
MIR	PLS	1456	pH^{A}, SOC^{B}, TN^{B}, P^{C}	[98]
MIR	PLS	307	pH^{A}, clay^{B}, sand^{B}, Mehlich-3(Al, Ca)^{A}, TC^{A}	[99]

MIR	PLS	270	Clay^{A}, sand^{A}, organic C^{B}, inorganic C^{A}	[106]
MIR	PLS	68	TC^{A}, SOC^{A}, TN^{C}, pH^{C}, sand^{C}, clay^{B}, silt^{B}	[101]
MIR	PLS	655	Lime Requirement (LR)^{A}	[93]

4.3. Comparative studies between the NIR and MIR spectroscopy

As summarized in **table 3,** several researchers compared the performance of the two infrared techniques MIR and NIR in addition to the fusion of the two techniques [109–125], for the prediction of one soil property [111,114,117,119,125,126] (e.g. **figure 4** that shows the results obtained by Viscarra Rossel et al. [126]), two soil properties [110,124] or multi-predictions [109,112,113,115,116,118,120–123]. The results and conclusions differ depending on the case and the properties to be predicted and the quality of predictions can be affected by many factors, Viz. the presence of some outliers, the existence of chemical compound that hide the bonds corresponding to the desired property (e.g. Carbonate ion mask the ones corresponding to the organic C) [127]. Some researchers concluded that MIR spectroscopy is the best [111,112,114,119–123,125], others prefer NIR [115], and several studies have shown that combining and merging the two datasets can significantly improve the predictions [113,116,124].

Figure 4 here

Figure 4. Partial least-squares regression modelling and prediction output for soil lime requirements (LR) for each of the VIS, NIR, MIR and VIS–NIR–MIR methods used. Columns: (a) shows the cross-validated root mean squared errors of prediction (RMSEP) against the number of factors (NF); (b) shows selection of the model with the fewest number of factors, such that the RMSE for this model is equal to, or not significantly larger than $RMSE_{ref}$. The level of significance used was $\alpha = 0.1$; and (c) shows the observed (y) against the cross-validated PLSR predictions ($\hat{Y}$) of soil LR with the validation statistics. Reused with permission [126]

Table 3. A summary of the recent studies that have compared the MIR and NIR techniques in combination with multivariate calibrations for the prediction of soil properties. A: well predicted ($R^2 > 0.8$), B: acceptable prediction ($0.6 < R^2 < 0.8$), C: poor prediction ($R^2 < 0.6$)

IR technique	Multivariate calibration	Sample size	Predicted properties	References
MIR vs NIR	PLS	111	$SOC^{A(NIR)}$, $pH^{A(NIR)}$, $As^{A(NIR)}$, $Cu^{A(NIR)}$, $Zn^{A(MIR)}$, $Pb^{B(NIR)}$, $Cr^{B(MIR)}$	[109]
MIR vs NIR	PLS	217	$SOC^{A(MIR)}$, $TN^{A(MIR)}$	[110]
MIR vs NIR vs MIR-NIR	PLS, SVMR	280	Available $N^{A(NIR)}$, $P^{A(MIR)}$, $K^{A(MIR)}$	[118]
MIR vs Vis-NIR	PLS, RF	305	$TC^{A(MIR, RF)}$	[119]
MIR vs Vis-NIR	PLS	--	(Clay, sand, silt)$^{B(MIR)}$, $TC^{A(MIR)}$, $TN^{A(NIR)}$, $C/N^{A(NIR-MIR)}$, $CEC^{A(MIR)}$, Exch (Ca, K, Mg, P, Cu, Fe, Mn, Na, Zn, Al, Si)$^{B(MIR)}$, $TP^{B(Vis-NIR)}$, $pH^{B(Vis-NIR)}$, $CaCO_3{}^{A(MIR)}$	[120]
MIR vs Vis-NIR	PLS	60	$SOC^{A(MIR)}$, $pH^{A(MIR)}$	[121]
MIR vs Vis-NIR	PLS	198	$CEC^{B(MIR)}$, $SOC^{A(MIR)}$, pH^{C}, $P^{B(MIR)}$, $exchCa^{B(MIR)}$	[122]

MIR vs Vis-NIR	SVMR	1259	$(pH(H_2O)$, sand, clay, TOC, CEC$)^{B(MIR)}$, P^{C}, K^{C}, (Ca, Mg, Al, Cu, Fe, Zn, Mn$)^{B(MIR)}$, B^{C}	[123]
MIR vs Vis-NIR	PLS, RF	1014	$TC^{A(VisNIR-MIR)}$, $SOC^{A(MIR)}$	[124]
MIR vs NIR	PLS	150	$TC^{A(NIR)}$	[125]
MIR vs Vis-NIR	PLS	3800	$SOC^{A(MIR)}$	[111]
MIR vs Vis-NIR	PLS	458	(pH, CEC, sand, clay, silt, Na, Ca, Mg$)^{B(MIR)}$, K^{C}	[112]
MIR vs NIR	PLS	2845	pH $(H_2O)^{B(MIR)}$, (TN, TC, Clay, sand, Silt, CEC$)^{B(NIR-MIR)}$, Exch(P, K, Ca, Mg, Na$)^{B(MIR)}$, S^{C}, Cu^{C}, Mn^{C}, $B^{B(NIR-MIR)}$, Zn^{C}, (Al, Fe$)^{B(NIR-MIR}$	[113]
MIR vs NIR	PLS	90	$SOC^{A(MIR)}$	[114]
MIR vs Vis-NIR	PLS	--	(N, P, K) $^{B(NIR)}$	[115]
MIR vs NIR vs MIR-NIR	PLS, CNN	14594	(pH, clay, sand, CEC, TC, SOC$)^{A(MIR)}$	[116]

MIR vs Vis-NIR	PLS	95	$SOC^{A(Vis\text{-}NIR)}$	[117]

4.4.Data preprocessing tools for soil properties prediction improvement

Spectral preprocessing techniques are mathematical transformations that aim to account for the noise in the spectrum or to eliminate some sources of variation that disturbs the prediction of the variables of interest, whether related to soil chemistry, physic or the biology of the analyzed samples. In the field of soil spectroscopy, several studies have been carried out to select the best preprocessing treatment to improve soil properties prediction. However, there is no general agreement about which pre-treatment is the most effective. Different options should be tested including the combination of several strategies of pre-treatment. [128] used the first-derivative transformation with a smoothing interval of 21 data points. [129] tested various transformations, each one having a specific effect: first-derivative transformation with a smoothing interval of 21 data points to minimize the variation in the data caused by sample grinding and optical setup, and the multiplicative scatter correction to correct the noise caused by the light scattering effects. [130] studied the effect of the six most used pretreatments, namely Savitzky–Golay smoothing, first derivative, log(1/R), mean centering, standard normal variate, and multiplicative scatter correction, the finding was that the first derivative transformation led to the best predictive models. [131] found that the first derivative preprocessing method gave the best results for the prediction of soil heavy metals, whereas multiplicative scatter correction and standard normal variate spectral preprocessing showed weak prediction for all the measured metals. [132]found that among the preprocessing techniques they studied, the scatter-correction group MSC and SNV showed improved prediction capability. [133] reduced the noise by smoothing the soil spectra using the Savitzky–Golay first-order polynomial across a moving window of five bands. Then, the first order detrending transformation was used to remove the baseline of the signals in the spectral data. This study confirmed the high potential of using spectral preprocessing techniques to predict soil properties. [38] proved that by combining more than one preprocessing strategy, namely, Savitzky–Golay smoothing with SNV and the first derivative yielded the best predictions of organic matter content in saline-alkali soils (**figure 5**).

Figure 5 here

Figure 5. Effect of applying different preprocessing techniques on predictive soil organic matter models based on Vis-NIR data. Reused with permission [38]

5. Conclusion & perspectives

This review has evidenced the effectiveness of infrared spectroscopy for soil characterization. Unlike the routine agrochemical analytical methods, which are time consuming, costly and which use hazardous chemical reagents, infrared spectroscopy is a rapid, inexpensive and eco-friendly alternative. Therefore, the advances in the instrumentation and the efforts to improve the machine learning and preprocessing tools should be considered as an opportunity to improve the effectiveness of these methods of diagnosis. In particular, the advances include the new generation of portable instrumentation available for the two discussed techniques (MIR and (Vis-)NIR) and the coupling of the generated spectral database with appropriate multivariate calibration strategies, which yield accurate predictions of several properties, especially when in-field measurements are needed.

Advanced multivariate models performed on infrared spectra in both ranges after applying appropriate data preprocessing tools can generate accurate predictions for most of the soil characteristics.

The studies cited in this paper showed that infrared spectroscopy especially in MIR led to predictive models that are able to give reasonable estimations of important key soil health indicators, namely, SOC, pH, sand, clay... etc. and offered several important advantages over the conventional soil laboratory methods where chemical reagents are ubiquitous.

The big challenges facing this new generation of dry chemistry laboratories are the model transfers from one instrument to another, between laboratories and countries. Future research must include as an important objective to standardize the working methods including the methods of sample preparation (drying and grinding), the spectral wave ranges (Vis-NIR, NIR, MIR) and even the brands of instruments used when scanning the samples. These efforts will undoubtedly contribute to solve the model transfer issue.

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Abbreviations

Soil Science:

AfSIS: Africa Soil Information Service

AS: Aluminum Saturation

B: Boron

C: Carbon

CEC: Cation Exchange Capacity

Cl: Chlorine

Cu: Copper

Al_{ex}: Exchangeable Aluminum

Fe: Iron

HWE-C: Hot-Water Extractable Carbon

IR: Infrared spectroscopy

K: Potassium

LR: Lime Requirement

Mn: Manganese

Mo: Molybdenum

N: Nitrogen

NIR: Near Infrared Spectroscopy

pH: potential Hydrogen

SOC: soil organic carbon

SOM: Soil organic matter

TC: Total carbon

TN: Total nitrogen

TP: Total Phosphorus

Vis-NIR: Visible and Near Infrared spectroscopy

Zn: Zinc

Chemometrics:

ANN: Artificial Neural Network

CCR: Correlated Components Regression

CNN: Conventional Neural Network

FD: First Derivative

GLSW: Generalized Least Squares Weighting

MC: Mean Centering

MIR: Mid Infrared Spectroscopy

MLR: Multiple Linear Regression

OSC: Orthogonal Signal Correction

PCA: Principal Components Analyses

PCs: Principal Components

PCR: Principal Components Regression

PLS: Partial Least Squares

PLS-NN: partial least-squares regression and neural networks

RF: Random Forest

RR: Regression Rules

SVMR: Support Vector Machine Regression

SG: Savitzky-Golay

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