Soil & Tillage Research 199 (2020) 104571

Contents lists available at ScienceDirect

Soil & Tillage Research

journal homepage: www.elsevier.com/locate/still

Using reflectance spectroscopy for detecting land-use effects on soil quality in drylands

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A R T I C L E I N F O

Keywords:
Land-use dynamics
Soil quality index
Partial least squares-regression
Partial least squares-discriminant analysis

A B S T R A C T

The rapid growth in the global population over the past few decades has resulted in the transformation of many natural ecosystems into human-dominated ones. Land-use (LU) dynamics are accompanied by an increase in resource exploitation, often causing deteriorated environmental conditions that are reflected in the soil quality. Soil quality differences between LUs can be observed and measured using near-infrared reflectance spectroscopy (NIRS) methods. The research goal was to apply, measure, and evaluate soil properties based solely on the spectral differences between both natural and human-dominated LU practices, in the dryland environment of the central Negev Desert, Israel. This goal was achieved through the development and implementation of chemometrics techniques that were generated from soil point spectroscopy. Soil quality index (SQI) values, based on 14 physical, biological, and chemical soil properties, were quantified and compared between LUs and geographical units across the study area. Laboratory spectral measurements of soil samples were applied. Significant differences in SQI values were found between the geographical units. The statistical and mathematical methods for evaluating the soil properties' spectral differences included principal component analysis (PCA), partial least squares-regression (PLS-R), and partial least squares-discriminant analysis (PLS-DA). Correlations between predicted spectral values and measured soil properties and SQI were calculated using PLS-R and evaluated by the coefficient of determination (R^2), the Root Mean Square Error of Calibration, and Cross-Validation (RMSEC and RMSECV), and the ratio of performance to deviation (RPD). The PLS-R managed to produce "excellent" and "good" prediction values for some of the soil properties, including EC, Cl, Na, Ca + Mg, SAR, NO_3, P, and SOM. Results of the PLS-R model for SQI are $R^2 = 0.90$, RPD = 2.46, RMSEC = 0.034, and RMSECV = 0.057. The PLS-DA classification of the laboratory spectroscopy was applied and resulted in high accuracy and kappa coefficient values when comparing LUs. In contrast, comparing the sampling sites resulted in lower overall accuracy (Acc = 0.82) and kappa values ($K_c = 0.80$). It is concluded that differentiation between physical, biological, and chemical soil properties, based on their spectral differences, is the key feature in the successful results for recognizing and characterizing various soil processes in an integrative approach. The results prove that soil quality and most soil properties can be successfully monitored and evaluated using NIRS in a comprehensive, non-destructive, time- and cost-efficient method.

1. Introduction

Global population growth over the past few decades has increased the need for food, shelter, and other services, and has resulted in the transformation of many natural ecosystems into human-dominated ones (Foley, 2005). Land-use (LU) change from natural to human-dominated land is a critical aspect of global change (Orenstein and Hamburg, 2009; Phillips et al., 2017) and may cause deteriorated environmental conditions (Metzger et al., 2006; Tscharntke et al., 2005). Such LU changes have enabled humans to increase needed resources, but they also potentially reduce the capacity of ecosystems to maintain food production and to regulate climate, soil, and air quality in a sustainable way. LU practices determine soil quality and soil function, which constitute crucial aspects for future sustainable LU management (Crist et al., 2017). Therefore, remediation and maintenance of the soil quality in response to LU is essential (Adeel et al., 2005), especially in drylands, where the soil undergoes degradation processes.

Assessment of soil quality includes the integration of physical, biological, and chemical properties as indicators of the soil's performance (Andrews et al., 2004). These key soil properties are dynamically

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https://doi.org/10.1016/j.still.2020.104571
Received 11 June 2019; Received in revised form 17 November 2019; Accepted 3 January 2020

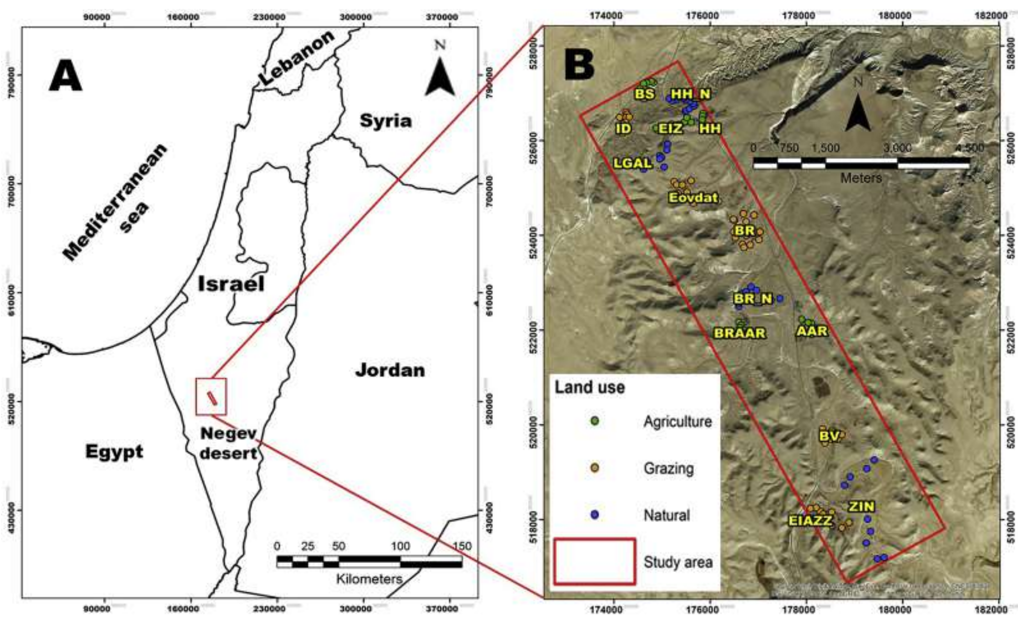

Fig. 1. (A) Location of the study area in the Negev Desert, Israel; (B) the selected study area with the sampling points of the three land-use categories (agriculture, grazing, and natural reserves), whose locations were selected from a prior stratified random methodology. Full names and number of soil samples for all sampling sites are presented in Table 1.

variable in space and time. Soil quality assessment can be applied to either human-dominated LUs, such as agriculture, where the primary ecosystem service is yield (agricultural productivity), or to natural ecosystems, where the primary ecosystem service could be the continuation of the environmental conditions and biodiversity conservation (Bünemann et al., 2018). The variability of soil indicators makes soil quality assessment a challenging task (Doran and Parkin, 1994). Two main approaches for this task are the Soil Management Assessment Framework (SMAF) (Andrews et al., 2004; Viscarra Rossel et al., 2006; Wienhold et al., 2009) and the Comprehensive Assessment of Soil Health (CASH) (Idowu et al., 2009; Moebius-Clune et al., 2016). Both approaches are based on selecting a Minimum Data Set (MDS), comprising a minimum number of indicators (soil properties) for defining and quantifying soil performance, while avoiding over-complexity of the soil quality assessment model and maintaining its reproducibility, ease of sampling, and low cost (Andrews et al., 2004; Karlen et al., 1997). According to Bünemann et al. (2018), SMAF is a more flexible framework in terms of selecting indicators using standardized protocols. Once the MDS is selected, the indicators are then transformed into a normalized score that represents the soil quality index (SQI) value (Andrews et al., 2004, 2002; Karlen et al., 1997). Soil quality assessment using the SQI method has been widely demonstrated in the literature, for both agricultural purposes (Mandal et al., 2001; Mukherjee and Lal, 2014; Triantafyllidis and Kontogeorgos, 2018) and ecological monitoring (Blecker et al., 2012; Lima et al., 2016; Paz-Kagan et al., 2016). In the case of ecological preservation, the SQI is not an absolute independent score, as it sets as an indicator for the degree of change in reference to the uninterrupted natural soil.

SQI requires extensive soil analyses, which remain expensive, as well as time and labor-consuming when using the standard procedures (Paz-Kagan et al., 2014). Therefore, more straightforward, time and cost-efficient, and non-destructive soil quality assessments are required. Near infrared reflectance spectroscopy (NIRS) grants the ability to assess various aspects of soil quality with non-destructive, reproducible, and cost-effective techniques. NIRS is based on hyperspectral data, including the visible (VIS, 400–700 nm), near-infrared (NIR, 700–1100 nm), and shortwave infrared (SWIR, 1100-2500 nm) spectral regions. Studies have shown the advantages of using RS in time-efficiency and the simultaneous analyses of multiple soil properties (Awiti et al., 2008; Cécillon et al., 2009; Romsonthi et al., 2018; Velasquez et al., 2005; Veum et al., 2017). Paz-Kagan et al. (2014) demonstrated the use of 14 soil quality indicators in the variability of soil attributes among three different LU types that changed from managed to unmanaged and vice versa. They developed the spectral soil quality index (SSQI) based on the NIRS of physical, biological, and chemical soil analyses. The SSQI integrates all relevant scored SQI indicators and then classifies them according to their soil spectral differences.

Although soil spectroscopy has been demonstrated successfully in many areas, these studies were mostly related to temperate climate regions that were subjected to anthropogenic effects, mainly agricultural systems, and were limited to a few land-use practices. The application of NIRS has not been previously applied in such hyper-arid environment. This is possibly due to the relatively small-scale human activity and LU changes that generally occur in such scarcely populated regions with extreme climatic conditions. Hence, the main goal of the current research is to assess the effect of LU alteration, with different management practices, on soil quality in a dryland area. The novelty of this research lies in applying the combined SQI and NIRS methods in a water-scarce and nutrient-poor arid area. This objective was accomplished by integrating physical, biological, and chemical analyses, as well as NIRS laboratory-derived data, followed by the SQI method, in the Avdat region, Israel. The research questions include: (1) How do the different management practices (LU) impact soil indicators in an arid area? (2) Which indicators are more sensitive to different management practices?, and (3) Can soil properties and SQI be predicted based on NIRS in arid soils?

2. Material and methods

2.1. Study area

In this study, the Avdat region, a scarcely populated dryland region in the Negev Desert of Israel, was selected. The area, which extends over 24 km^2, was chosen since it includes two main human activities, crop cultivation (mainly vines and olives) and the grazing of goats and sheep, that are adjacent to natural park reserves with unique ecological values (Ohana-Levi et al., 2018). The study area (Fig. 1) contains three LU categories, including two types of settlements: agricultural farms (single-family), agro-pastoral grazing land (Bedouin villages), and natural park reserves. The area is defined as arid by the aridity index (UNEP, 1992), which is calculated by the ratio between the annual rainfall (80–100 mm) and the annual potential evaporation (about 1700 mm), in which the precipitation gradient decreases and the evaporation rate increases the further southward from the Mediterranean

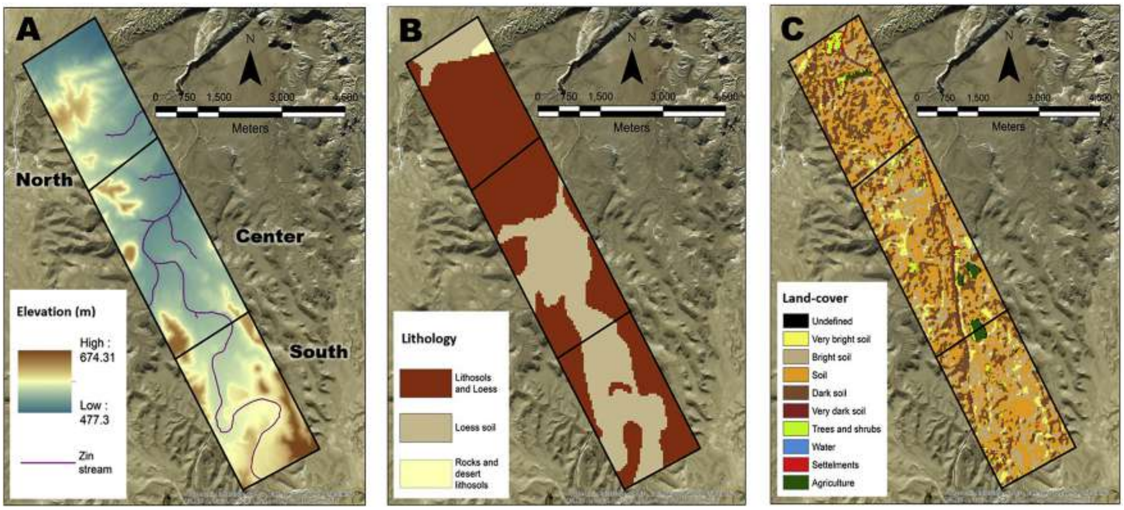

Fig. 2. Stratified random survey components of Avdat region: (A) elevation, (B) lithology, (C) land use-land cover (LULC) classification, and the study area's geographical units: north, center, and south.

Table 1

Distribution of 121 soil samples among 14 sites across the Avdat region. Each site includes several samples, land-use type (agriculture, grazing, or natural), topographic landscape position and mean elevation, and soil class based on mean fractional soil texture.

Sampling site	Number of samples	Land use type	Landscape position and elevation (m)	Soil class and mean fractional Sand, Silt, and Clay (%)
Even Ari farm (AAR)	6	Agriculture	Toeslope (547)	Loam (40.13, 46.2, 13.67)
Borot Ramaliah (BR)	16	Grazing	Toeslope (528)	Sandy Loam (63.1, 23.1, 13.8)
Borot Ramaliah-Even Ari (BRAAR)	6	Agriculture	Toeslope (527)	Loam (51.83, 31.47, 16.7)
Borot Ramaliah natural (BR_N)	9	Natural	Valley, Channel (523)	Sandy Loam (62.7, 23.17, 14.13)
Beit Hashanti (BS)	13	Agriculture	Toeslope, Valley (510)	Sandy Loam (53.17, 27.67, 19.16)
Bedouin village by Even-Ari (BV)	5	Grazing	Toeslope, Valley (559)	Sandy Loam (61.4, 23.6, 15)
El Azazme-Hava stream (EIAZZ)	9	Grazing	Footslope, Toeslope (572)	Sandy Loam (66.4, 17.86, 15.74)
Eyal Israeli farm (EIZ)	8	Agriculture	Footslope (549)	Sandy Loam (58.43, 27.82, 13.75)
Ein Avdat (Eovdat)	9	Grazing	Footslope, Toeslope (541)	Sandy Loam (56.87, 25.52, 17.61)
Havarim stream (HH)	4	Agriculture	Toeslope (553)	Sandy Loam (61.3, 24.7, 14)
Havarim stream natural (HH_N)	10	Natural	Backslope, Footslope (524)	Sandy Loam (60, 30.2, 9.8)
Bedouin village by Beit Hashanti (ID)	8	Grazing	Toeslope (525)	Sandy Loam (62.15, 23.52, 14.33)
Lifa gal viewpoint (LGAL)	8	Natural	Summit (597)	Sandy Loam (58.49, 24.7, 16.81)
Zin stream (ZIN)	10	Natural	Toeslope, Channel (592)	Sandy Loam (59.22, 25.37, 15.41)

Sea (Ziv et al., 2014). The average daily temperature ranges from 5 °C in the winter to 32 °C in the summer (Olsvig-Whittaker et al., 2012). Lithology is dominantly characterized by limestone mixed with dolomite, chalk, and marl. The soil type in the area is homogeneous, consisting mostly of loess soil (Ohana-Levi et al., 2018). Soil development occurs mostly in the upper parts of the watershed, where shallow patches of soil cover exist among steep barren limestone rocks, and in the lower parts, which consist of colluvium embedded with unconsolidated rocks. The soil columns range from 80 cm in the upstream part to several meters in the lower parts (Olsvig-Whittaker, 1983; Yair and Danin, 1980).

2.2. Soil sampling

The sampling area included 14 different sites within the three LUs. Selecting the precise soil sample locations was done by conducting a prior stratified random methodology (SRM, Fig. 2) that was based on three different inputs: (1) elevation based on a digital elevation model; (2) soil type based on a pedology map, with the spatial distribution of soil texture from the official Survey of Israel data; and (3) LU categories based on the classification of a Landsat 8 image acquired on 13 August 2016, with an overall accuracy of 99.8% (Ohana-Levi et al., 2018). The SRM allows the selection of random soil samples based on the variation of the different data sources (Kothari, 2004).

2.3. Geographic units and laboratory analysis

Since the study area stretches over a broad and elongated cross-section of approximately 11 km in length (Fig. 1), with different elevations and climatic attributes, soil indicator values may present some significant differences within the study area that are more related to the environmental gradient than to LU management practices. For example, elevation gradually increases southwards (Fig. 2A), whereas the northern and central parts share a relatively flatter surface around the Zin's downstream basin. Lithology differs as well (Fig. 2B), in which smoother loess soils reside around the stream path. Evapotranspiration, combining precipitation and temperature as environmental factors, shows significant differences between all three parts, in which the mean annual rates are 1671, 1694, and 1717 mm for the northern, center, and southern sections, respectively. Therefore, the statistical analysis was divided into three geographical units to minimize the environmental effect and to evaluate the management practices' effects on soil quality.

Soil samples from the different management practices were collected and transferred to the laboratory for physical, biological, and chemical soil analysis and laboratory spectroscopy. A total number of 121 soil samples were collected in April 2017 from 14 different sites scattered across the landscape. These are presented in Table 1 with their respective LU, landscape position, elevation, soil class, and texture. The soil samples were collected from the upper topsoil at a depth of 0–15 cm, mostly from lower topographical locations around low-

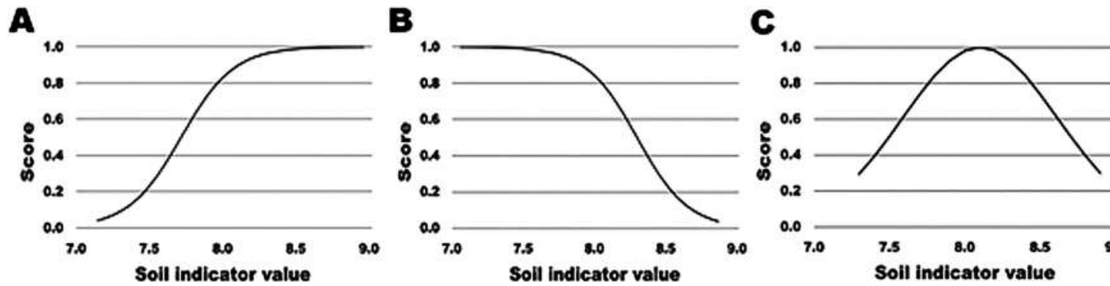

Fig. 3. Examples of scoring curves of the respective transformation functions: (A) more is better, (B) less is better, and (C) optimum.

slopes and stream basins, where the soil column is more developed. Each soil sample was assigned an accurate location using a portable GPS device. The soil samples were packed into paper bags, then transferred and stored unopened at room temperature until analysis and laboratory survey.

The analytic methods included 14 analyses based on the SMAF protocol (Wienhold et al., 2009): physical: soil texture (fractional clay, silt, and sand) for assessing the soil structure and fragmentation, and the available water content (AWC), related to the plant available water storage capacity; biological: soil organic matter (SOM), related to energy and nutrient storage and carbon sequestration, and extractable nitrate (NO_3^-) in the soil, related to nitrogen-containing life building blocks and nitrogen release; and chemical: pH, electrical conductivity (EC), extractable chlorine (Cl), extractable sodium (Na), extractable calcium and magnesium (Ca + Mg), and the sodium adsorption ratio (SAR), which act as indicators for soil salinization condition, and extractable phosphorus (P) and extractable potassium (K), which are essential nutrients, available in the soil, for plant growth and health.

The measurement of AWC was conducted by oven-drying the soil samples at 105 °C to a constant weight, followed by measuring the weight differences (Scrimgeour, 2008). Soil organic matter (SOM) was measured by the organic carbon-furnace method after oven-drying soil samples at 105 °C for 3 h (to remove any $CaCO_3$) and weighing the soil samples, followed by burning the dry soil in a furnace for 2 h at 500 °C and re-weighing the soil samples (Casida et al., 1964). Soil nitrogen (N) was measured as extractable nitrate (NO_3^-) by potassium chloride extractions (Norman and Stucki, 1981). Soil nutrient values (NO_3^-, P, K, Na, Ca, Mg) were extracted by shaking an ammonium acetate plus acetic acid solution with pH 4.8, which was then filtered through paper, and analyzed using an inductively coupled plasma emission spectrometer (ICP) (Weil and Brady, 1999). The samples' pH values were measured by composing a 2:1 part water-soil suspension and determined using the pH electrode probe of a Lignin pH robot. Finally, the soil EC was examined on a well-stirred 1:1 soil-water suspension (20 ml each), using an EC meter.

2.4. Spectral measurement and processing

The spectral measurements of all 121 soil samples were performed in laboratory conditions. The soil samples were sieved through a 2-mm sieve to remove aggregation and stones and were spectrally measured using the portable Analytical Spectral Devices (ASD) Field Spec® Pro spectrometer. The ASD spectral range is 350–2500 nm with a 25° field of view. The spectrometer was recalibrated using a standard white reference panel (Spectralon Labsphere Inc., North Sutton, NH, USA). Samples were scanned under illumination from four directions, while the spectrometer sensor was set above the sample at the height of 18.5 cm. The idea behind this step is to diminish the effects of microtopography shadowing (bidirectional illumination effects). The mean value of every four readings was used as the representative sample signature that was then averaged to one spectral reading. The spectral resolution of the obtained data was 1 nm for the entire spectral range.

2.5. Development of soil quality index (SQI)

Soil quality indices combine all relevant indicators for soil condition interpretation within a proportional score. Transforming the indicators is necessary in order to standardize each indicator on a comparable scale. All indicators from the laboratory analysis were transformed and standardized into unitless scores (Si), ranging from 0 to 1, which were then given a proportional weight and summed. These scores represented each of the indicator's explanatory contributions to the soil conditions according to management practices and LU, where natural ecosystem measurements were set as a reference for the other two LUs. AWC, SOM, and NO_3^- are essential soil quality indicators. Therefore, the maximum presence of all indicates higher soil quality.

On the other hand, high abundances of EC, Cl, Na, and Ca + Mg soil properties may indicate a condition in which the soil is under salinization process, which means lower soil quality and functionality. Therefore, the aim is to observe lower soil salinity values. The remaining soil indicator values (pH, SAR, P, and K) are likely to vary between each LU treatment, where either very high values (e.g., excessive fertilizing) or low ones may harm the soil's quality. Hence, an equal amount needs to be obtained. The sampling sites were grouped according to their geographical locations (i.e., northern, central, and southern), and their overall SQI values and physical, biological, and chemical components were calculated separately.

Eqs. 1–3 and Fig. 3 show the scoring functions, including their respective typical curves, according to the above adjustments and transformations, and based on previous literature (Moebius-Clune et al., 2016; Paz-Kagan et al., 2014; Seybold et al., 1997; Wienhold et al., 2009). Three functions can be defined: (1) the "more is better" scoring curve with positively graduating slopes that characterize AWC, SOM, and NO_3^-; (2) the "less is better" curve for negatively depressing slopes, which represents EC, Cl, Na, and Ca + Mg; and (3) the "optimum" curve that centers around a mean value, which characterizes pH, SAR, P, and K. The transformations of the original values were calculated using the following functions (Masto et al., 2007):

$$Si_{more} = \frac{1}{1 + b^{-b(x-a)}} \tag{1}$$

$$Si_{less} = \frac{1}{1 + e^{b(x-a)}} \tag{2}$$

$$Si_{optimum} = 1 \times e^{\frac{-(x-a)^2}{b}} \tag{3}$$

where x is the soil property value, a is the value's least square deviation from the mean, and b is the slope of mean according to its standard deviation ($2d^2$). Soil indicator performances with scores from 1.0–0.8 are considered to be very high scores, 0.8–0.6 are high, 0.6–0.4 are medium, 0.4–0.2 are low, and 0.2–0.0 are very low scores.

Once the original values were rescaled by their respective functions, a principal component analysis (PCA) was performed for further interpretation. The PCA is a statistical method that aims to reduce the number of dimensions within a dataset (Jolliffe and Cadima, 2016). It transforms correlated variables into a smaller number of significantly different uncorrelated dimensions (variables) called principal components (PC), where the chosen number of PCs account for most of the variability of the data (Hotelling, 1933). The low co-variability among PCs helps to separate the data into statistically distinct groups. For this reason, the correlations between variables were calculated. Soil variables that were highly correlated were removed from the data to prevent redundancy in the model (Jolliffe and Cadima, 2016). PCs with a higher proportion of variance than 5% were examined. The scored soil properties were calculated into an additive value of the essential weighted indicators for each LU, which is the ultimate soil quality index (SQI) Eq. (4):

$$SQI = \sum_{i=1}^{n} PWi \times Si' \tag{4}$$

where PWi is the PCA weighing factor and Si' is one of the scoring functions, depending on the soil property. This final index value is considered as a total rank of the soil quality, with regard to the examined management practices and LU under study.

2.6. Correlation and classification of soil and spectroscopy analysis

The correlation between the laboratory soil measurements and their spectral data was performed using a partial least squares-regression (PLS-R) cross-validation procedure. PLS-R is a predictive technique for quantitative spectral analysis (Paz-Kagan et al., 2014; Viscarra Rossel et al., 2006). Its main advantage derives from its ability to use multiple predictor variables to create predictive models with high collinearity. PLS-R uses covariance between the spectra (predictor: X) and the soil laboratory analysis, as well as the SQI (response variables: Y). The focus was placed on the abovementioned soil indicators and their correlations with their spectral data. Each soil indicator correlates differently with its spectral reading, and each has more significant wavelengths with which it corresponds. This is due to the fact that characteristic wavelengths differ between each soil indicator and management practice according to the relationship their physical and chemical structures maintain with the electromagnetic radiation, which can be measured in a comparative spectral analysis (Ben-Dor et al., 2009; Cécillon et al., 2009).

Pre-processing transformations (PPTs) were applied and tested on the spectral signatures in an attempt to improve their prediction ability through the regression process. Such PPTs include mean and maximum normalization and baseline offset effects corrections (Tekin et al., 2014), first and second derivatives of the reflectance values (Fystro, 2002; Shepherd and Walsh, 2002), the second-order polynomial Savitzky–Golay smoothing algorithm with 11 smoothing points (Savitzky and Golay, 1964), and generalized least squares weighting (GLSW) (Martens et al., 2003). The best predictive fitted values were found with the combination of two PPTs: (1) autoscale and (2) GLSW with a single adjustable parameter, α, which was set to 0.02 (Paz-Kagan et al., 2015; Rozenstein et al., 2015) (See Appendix A). To measure the relative importance of each wavelength, variable importance in projection (VIP) scores were derived from the PLS-R to determine the significant effect of each wavelength defined by each soil indicator. Evaluations of the prediction rate for the regressions between the predicted and observed soil indicators were made by calculating the Root Mean Square Error of Calibration and Cross Validation (RMSEC and RMSECV) and the coefficient of determination (R^2) values. Therefore, the data needed to be divided into a calibration dataset (75% of the data) and a randomly chosen validation dataset (25% of the data), which was used as the model prediction accuracy. In addition, to standardize the prediction correlations comparably, the ratio of performance to deviation (RPD) was calculated as RPD = SD/RMSECV. Chang et al. (2001) proposed the RPD's graduated ranking of the prediction models, in which models with RPD ≥ 2.5 and $R^2 \geq 0.80$ are considered "excellent," 2 < RPD ≤ 2.5 and $R^2 \geq 0.70$ are considered "good," 1.5 < RPD ≤ 2 and $R^2 \geq 0.60$ are considered "moderate," and RPD ≤ 1.5 and $R^2 < 0.60$ are considered "poor". However, Mcbratney and Minasny (2013) have warned about the use of both measures as the only indices of the prediction model, since they share a strong relationship and ultimately present the same concept. Thus, RPD and R^2 cannot be used as assessment tools for goodness of fit on their own. Instead, both measures should be presented and compared along with the RMSEC and RMSECV of the prediction models to compare the models' prediction intervals.

Assessment and quantification of the differences in the spectral variation in soil quality between LUs were conducted using partial least-squares discriminant analysis (PLS-DA). The PLS-DA categorizes the continuous predictor variable (X: soil indicators) into separate classes according to their variance between each group of samples. The outcome of the PLS-DA is a scatterplot in which each sample is classified into one of the predetermined classes (LU or sampling site), in addition to a statistical evaluation of significant differences between classes.

2.7. Statistical analysis of soil properties and SQI

We applied a one-way analysis of variance (ANOVA) for each soil indicator and SQI under each particular LU. The distinction between each pair of LUs made by their separation of means was examined using a Tukey Honest Significance Difference (HSD) post hoc test, for which $p \leq 0.05$ indicates a significant difference. In cases where ANOVA assumptions of the variables were not met for the original data, a logarithmic transformation was applied, followed by a reexamination of the assumptions. If the indicators' assumptions were still violated, a non-parametric Kruskal-Wallis test was conducted, following by a pairwise Wilcoxon rank-sum test to examine significant differences between pairs of LUs for each soil property. Statistical calculations and analyses were performed using the R-Studio version 1.0.143 software (RStudio Inc., Boston, MA, USA).

3. Results

3.1. Soil property analysis

The laboratory analysis of the soil is shown in Table 2, presenting the mean values of the soil properties and their standard deviations (SDs), according to their LU and geographical unit. To remove the minimum number of outliers from the dataset, by excluding only the extreme values, we applied the median absolute deviation (MAD) approach that excludes observations higher or lower than three SDs around the variable's median value (Leys et al., 2013). Using the MAD method on the data resulted in the removal of very few outliers, not exceeding 5% removal for any of the soil properties; for some soil properties, no outliers were removed. Fig. 4 shows the comparative analysis of soil properties for the whole study area, without the geographical subdivision. In this case, only small significant differences were noticed between LUs. The soil texture analysis resulted in the classification of almost all the sampling sites as the sandy-loam soil type (Table1), according to the USDA soil texture triangle (Groenendyk et al., 2015), with a few soil samples classified as loam. Similar results were found when comparing LUs across geographical units (Table 2). One-way ANOVA tests for the original values showed that AWC and pH had no assumptions violated, and both showed no significant differences between LUs. Following this, the transformed data resulted in SAR and SOM properties having no assumptions violated and presenting some significant differences between LUs, according to the Tukey HDS test, in which for both indicators, the natural ecosystem LU showed lower values than the other two LUs with significant differences. For most soil properties, the agro-ecosystems and grazing LUs showed significantly higher values than those of the natural ecosystem, notably EC, Cl, Na, and Ca + Mg, which may indicate soil salinity levels.

Furthermore, the natural ecosystem showed significantly lower soil nutrient values (NO_3, P, and K) than the grazing and agro-ecosystem LUs, which implies the presence of higher biotic activity (due to

Table 2
The mean values of each soil property along with its respective land-use and geographical unit: (A) agro-ecosystems; (B) grazing; and (C) natural ecosystems, each presented with its standard deviation and significant differences between treatments, represented with small letters (a, b, c).

Soil Properties	Location	Natural ecosystems	Grazing	Agro-ecosystems
AWC (%)	North	37.07 ± 3.27[a]	39.6 ± 6.55[a]	35.04 ± 4.06[a]
	Center	34.24 ± 5.53[b]	35.96 ± 5.48[b]	40.83 ± 4.58[a]
	South	33.71 ± 5.43[a]	38.95 ± 7.72[a]	–
pH	North	8.08 ± 0.26[a]	8.1 ± 0.40[a]	7.99 ± 0.39[a]
	Center	8.01 ± 0.24[b]	7.96 ± 0.41[b]	8.3 ± 0.13[a]
	South	8.55 ± 0.28[a]	8.05 ± 0.27[b]	–
EC (dS/m)	North	5.82 ± 7.33[b]	13.58 ± 24.31[a]	25.85 ± 29.64[a]
	Center	3.21 ± 3.26[b]	16.8 ± 1954[a]	0.75 ± 0.15[c]
	South	9.22 ± 18.81[b]	18.54 ± 22.1[a]	–
Cl (mg/l)	North	45.83 ± 81.66[b]	147.89 ± 309.15[a]	296.75 ± 358.69[a]
	Center	23.65 ± 27.21[b]	171.05 ± 228.55[a]	1.45 ± 0.71[c]
	South	88.78 ± 201.25[b]	190 ± 275.17[a]	–
Na (mg/l)	North	29.86 ± 44.46[b]	79.66 ± 162.33[a]	103.32 ± 150.45[a]
	Center	21.2 ± 26.04[b]	103.78 ± 145.91[a]	1.21 ± 0.78[c]
	South	79.74 ± 177.49[a]	104.11 ± 150.63[a]	–
Ca + Mg (mg/l)	North	34.8 ± 44.21[b]	56.02 ± 81.62[b]	139.75 ± 162.02[a]
	Center	9.46 ± 8.05[b]	84.3 ± 99.9[a]	5.45 ± 1.7[b]
	South	28.22 ± 51.86[b]	67.37 ± 74.96[a]	–
SAR	North	3.37 ± 2.18[b]	13.46 ± 12.71[a]	4.9 ± 4.01[b]
	Center	2.86 ± 1.45[b]	6.48 ± 5.73[a]	8.33 ± 3.1[a]
	South	6.52 ± 10.28[b]	22.06 ± 18.64[a]	–
NO_3 (mg/kg)	North	34.58 ± 41.21[b]	93.51 ± 111.76[a]	143.37 ± 154.91[a]
	Center	26.92 ± 30.64[b]	94.62 ± 109.98[a]	14.82 ± 7.63[c]
	South	100.07 ± 220.28[b]	219.34 ± 193.783[a]	–
P (mg/kg)	North	9.53 ± 3.14[b]	56.52 ± 52.91[a]	13.62 ± 10.19[b]
	Center	13.55 ± 8.62[b]	31.68 ± 48.5[a]	17.87 ± 3.91[b]
	South	13.57 ± 5.37[b]	66.86 ± 51.62[a]	–
K (ml/kg)	North	0.5 ± 0.33[c]	6.41 ± 11.34[a]	2.1 ± 4.03[b]
	Center	0.42 ± 0.15[b]	3.1 ± 5.17[a]	0.48 ± 0.25[b]
	South	0.99 ± 1.41[b]	15.11 ± 17.71[a]	–
SOM (%)	North	1.61 ± 0.8[b]	3.18 ± 1.48[a]	3.17 ± 1.35[a]
	Center	1.94 ± 0.3[b]	2.59 ± 0.7[a]	2.44 ± 0.47[a]
	South	1.35 ± 0.51[b]	2.62 ± 1.61[a]	–
Sand (%)	North	59.32 ± 11.7[a]	59.35 ± 7.31[a]	56.15 ± 9.06[a]
	Center	62.7 ± 6.01[a]	63.1 ± 8.19[a]	45.98 ± 11.31[b]
	South	59.22 ± 16.46[a]	64.61 ± 7.03[a]	–
Silt (%)	North	27.75 ± 10.51[a]	24.58 ± 6.44[a]	27.24 ± 8.74[a]
	Center	22.86 ± 3.73[b]	23.1 ± 10.08[b]	38.83 ± 11.52[a]
	South	25.37 ± 14.89[a]	19.9 ± 5.45[a]	–
Clay (%)	North	12.91 ± 6.4[a]	16.06 ± 3.8[a]	16.6 ± 6.22[a]
	Center	14.43 ± 5.3[a]	13.8 ± 4.66[a]	15.18 ± 3.72[a]
	South	15.41 ± 6.4[a]	15.47 ± 3.41[a]	–

Note: AWC: available water content; EC: electric conductivity; Cl: chlorine; Na: sodium; Ca + Mg: calcium and magnesium; SAR: sodium adsorption ratio; NO3: nitrate; P: phosphorus; K: potassium SOM: soil organic matter; significant differences between land uses are marked with small letters, in which values in each column with the same letter do not differ significantly when $p < \alpha$ (0.05), using ANOVA and Kruskal-Wallis analyses followed by Tukey and Wilcoxon tests. A: high values; b: medium values; c: low values.

cropping and herding) in the soil of the latter two LUs. Nevertheless, the geographical subdivision emphasizes variations even better, where significant differences were shown between LUs for almost all soil indicators (Table 2). A significant difference was noticed between the agro-ecosystem sites (located only in the northern and central areas), for which much higher values were measured in the northern fields than in the central ones for both salinity (EC, Cl, Na, Ca + Mg, and SAR) and soil nutrient (NO_3, P, and K) indicators. The same soil properties, as well as the SOM, showed significantly higher values for the grazing and agro-ecosystem LUs than the natural ecosystem one. Moreover, significantly higher AWC was found in the central agricultural LU than in the other LUs.

Pearson correlation coefficients (r) for the given soil indicators were calculated and are presented in Table 3. To understand the relations and to consider the more powerful correlations between properties, significant correlations ($r \geq 0.5$) are marked in bold, and strong correlations ($r > \pm 0.8$) are marked in bold and with an asterisk (*). Multivariate correlations were also generated to avoid redundancy of properties. Very strong correlations were found between EC and Cl, Na, and Ca + Mg ($r = 0.99$, $r = 0.95$ and $r = 0.93$; $p < 0.01$, respectively), between Cl, Na, and Ca + Mg ($r = 0.94$ and 0.93; $p < 0.01$, respectively), between Na and Ca + Mg ($r = 0.86$; $p < 0.01$), and between sand and silt ($r = -0.88$; $p < 0.01$).

3.2. Soil quality index (SQI)

The SQI for each soil sample and their respective physical, biological, and chemical components was developed using the scores of the transformed soil properties' values. The soil texture variables (fractional sand, silt, and clay) and Cl, Na, and Ca + Mg (which are essential indicators for soil salinity) were excluded from the SQI and PCA calculations due to high collinearity and possible model redundancy (Jolliffe and Cadima, 2016). The PCA results showed that only three PCs had eigenvalues greater than 1 that explained 72.70% of the total cumulative variance of the original data (Table 4). PC1 accounts for 35.83% of the total variance and includes the pH, EC, and NO_3 soil properties. For PC2, the contributory variance was 22.29%, and includes the AWC and P indicators. The third PC3, with a response to 14.58% of the variation, contains SAR, K, and SOM soil indicators within 10% of the highest loading values.

The SQI scores and their physical, biological, and chemical components for all three LUs are shown in Fig. 5. The mean overall SQI

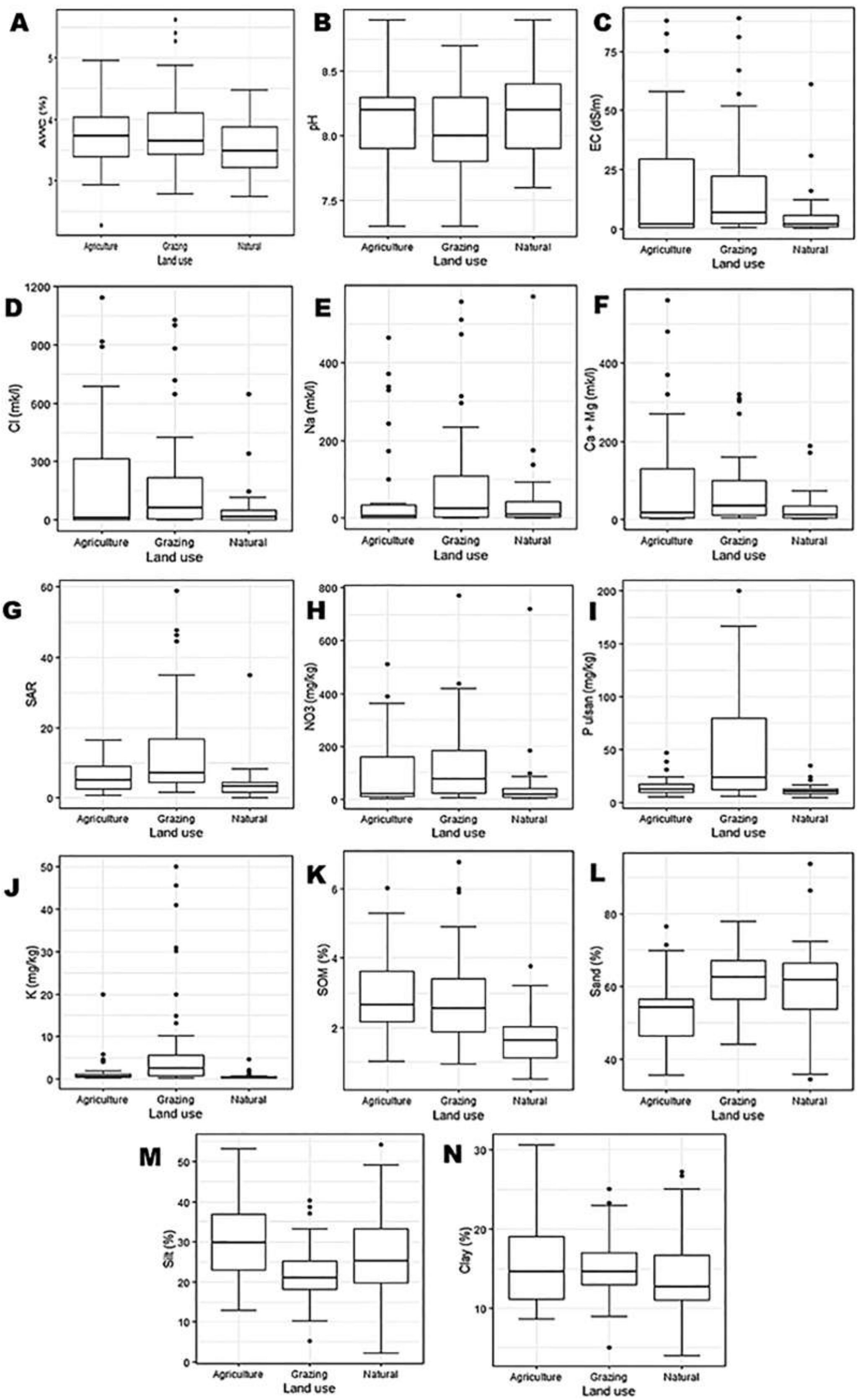

Fig. 4. Boxplot representation of each soil indicator value under different land uses of the entire study area: agriculture, grazing, and natural. Note: available water content (AWC); electrical conductivity (EC); extractable chlorine (Cl); extractable sodium (Na); extractable calcium and magnesium (Ca + Mg); sodium adsorption ratio (SAR); extractable nitrate (NO_3); extractable phosphorus (P); extractable potassium (K); and soil organic matter (SOM).

Table 3
A matrix presenting the measured soil quality properties and their respective Pearson correlation coefficients for the study area. Correlations with highly significant differences of $p \leq 0.05$ are marked in bold, whereas strong correlations ($R \geq 0.8$) with very highly significant differences of $p \leq 0.01$ were marked with (*).

	AWC (%)	pH	EC (dS/m)	Cl (mg/l)	Na (mg/l)	Ca + Mg (mg/l)	SAR	NO_3 (mg/kg)	P (mg/kg)	K (mg/kg)	SOM (%)	Sand (%)	Silt (%)	Clay (%)
AWC (%)	1.00													
pH	0.09	1.00												
EC (dS/m)	−0.20	**−0.55**	1.00											
Cl (mg/l)	−0.16	**−0.55**	**0.99***	1.00										
Na (mg/l)	−0.23	**−0.42**	**0.95***	**0.94***	1.00									
Ca + Mg (mg/l)	−0.19	**−0.56**	**0.93***	**0.93***	**0.86***	1.00								
SAR	**0.44**	−0.14	0.14	0.14	0.11	0.04	1.00							
NO_3 (mg/kg)	−0.09	**−0.41**	**0.76**	**0.71**	**0.74**	**0.67**	**0.31**	1.00						
P (mg/kg)	0.29	−0.24	0.06	0.05	0.01	0.001	**0.41**	0.19	1.00					
K) mg/kg)	0.12	−0.3	0.27	0.24	0.26	0.2	**0.47**	**0.55**	**0.46**	1.00				
SOM (%)	0.42	−0.38	**0.53**	**0.54**	**0.36**	**0.48**	0.39	0.39	0.38	0.33	1.00			
Sand (%)	−0.02	−0.1	0.001	−0.02	0.02	−0.06	0.17	0.03	0.17	0.14	−0.06	1.00		
Silt (%)	0.08	0.12	−0.05	−0.04	−0.13	0.01	−0.16	−0.13	−0.17	−0.16	−0.03	**−0.88***	1.00	
Clay (%)	−0.12	−0.03	0.11	0.12	0.22	0.1	−0.02	0.18	−0.02	0.03	0.19	−0.34	−0.15	1.00

Note: AWC: available water content; EC: electric conductivity; Cl: chlorine; Na: sodium; Ca + Mg: calcium and magnesium; SAR: sodium adsorption ratio; NO3: nitrate; P: phosphorus; K: potassium SOM: soil organic matter.

Table 4
Results of the principal component analysis (PCA) of soil in the study area. Chosen principal components' (PCs) scores for the model and their ranks are marked bold.

	Scores PC1	Scores PC2	Scores PC3
Eigenvalue	2.86	1.78	1.16
Variance (%)	35.83	22.29	14.58
Cumulative variance (%)	35.83	58.12	72.70
AWC (%)	0.06	**0.55**	0.42
pH	**0.38**	0.15	−0.23
EC (dS/m)	**−0.46**	−0.34	0.17
SAR	−0.19	0.41	**−0.43**
NO_3 (mg/kg)	**−0.50**	−0.18	−0.20
P (mg/kg)	−0.25	**0.51**	−0.008
K) mg/kg)	−0.39	0.20	**−0.40**
SOM (%)	−0.34	0.16	**0.57**

Note: AWC: available water content; EC: electric conductivity; SAR: sodium adsorption ratio; NO_3: nitrate; P: phosphorus; K: potassium SOM: soil organic matter.

scores in the northern part are SQI = 0.65, 0.61, and 0.66 for the agricultural, grazing, and natural LUs, respectively. None of the three LUs were found to be significantly different from each other ($\chi^2_{(2)} = 1.53$, $p = 0.46$). Both the biological (representing the SOM and NO_3 soil properties) and the chemical components of the SQI for the natural area differed significantly from the rest, with lower SOM and NO_3 components and higher values for the chemical properties. In the central part, the mean overall SQI scores were SQI = 0.72, 0.65, and 0.63 for the agricultural area, grazing, and natural LUs, respectively, with significant differences between all LUs for both overall SQIs and their components ($\chi^2_{(2)} = 15.67$, $p < 0.05$). The remaining southern part resulted in mean overall SQI scores of SQI = 0.61 and 0.59 for the grazing and natural LUs, respectively, with no significant differences. Within the southern SQI's components, only the biological showed significant differences.

3.3. Soil properties and SQI correlations with soil spectroscopy

The results of the PLS-R analysis are presented in Table 5. The results also include several latent variables (LV), coefficient of determination (R^2), RMSEC, RMSECV, RPD, and significant VIP bands used for each soil property included in the model. Soil properties with excellent (RPD ≥ 2.5 and $R^2 \geq 0.80$) and good (2 < RPD ≤ 2.5 and $R^2 \geq 0.70$) prediction scores are marked in bold and underlined in Table 5 and presented in Fig. 6, and include EC, Cl, Na, Ca + Mg, SAR, NO_3, P, and SOM. Fig. 6 also presents each soil property and SQI soil-laboratory versus soil-spectroscopy regression scatterplots, including their respective RMSEC, RMSECV, R^2, LVs, and RPD values. The overall SQI resulted in a good prediction value ($R^2 = 0.903$, RPD = 2.46, RMSEC = 0.034, and RMSECV = 0.057). The significant diagnostic wavebands were calculated and identified by the VIP for each soil property and SQI value. For example, significant scores for the highly correlated soil salinity properties (EC, Cl, Na, Ca + Mg, and SAR) were found within the range of bands with strong peaks at 1363, 1896–1899, 1982–1984, 2266–2270, and 2346 nm. Sensitivity bands for biological properties, such as SOM, were found across the VIS-NIR-SWIR regions, with significant peaks at 590–739, 853, 1364, 1899, 2014, 2203, and 2317 nm. For NO_3–, the wavebands centered mostly within the SWIR region, peaking at 652, 1361, 1420, 1773, 1901, 1974, and 2346 nm. The SQI, combining attributes from multiple soil indicators, found strong sensitivity at 1434, 1749, 1841, 1901, 1988, and 2343 nm.

3.4. Spectral classification of soil samples across LUs and sampling sites

The classification of the soil samples' spectral signatures across varied LUs and sampling sites is shown in Fig. 7, as well as the number of LVs, overall accuracy, and Kappa coefficient values. The PLS-DA classification across different LUs (Fig. 7A) resulted in high overall accuracy and Kappa coefficient values for both grouping methods. The separation between sampling sites (Fig. 7B) resulted in lower classification values, with an overall accuracy of 0.823, and a Kappa value of 0.802. In terms of classification capabilities, the PLS-DA is an accurate quantitative and qualitative approach for predicting variability between different LUs, and between sites to a slightly lesser extent.

4. Discussion

The effect of LU activity on soil was detected, quantified, and evaluated through a soil survey and spectral analysis of different soil indicators for comparing soil properties across different land practices. This research integrated both methods by applying the NIRS method to explain variations among LUs. The use of the NIRS approach for soil quality assessment in an arid area, such as the Avdat region in the Negev Desert, has been limited. Significant differences between LUs and sampling sites were found for almost all soil indicators and SQIs, for laboratory analyses, soil spectral measurements, and their integration with NIRS. The correlation values between measured and predicted SQI values was $R^2 = 0.903$, RPD = 2.46, RMSEC = 0.034, and RMSECV = 0.057. Spectral classifications resulted in high accuracy when segregating LUs, and with relatively lower values when

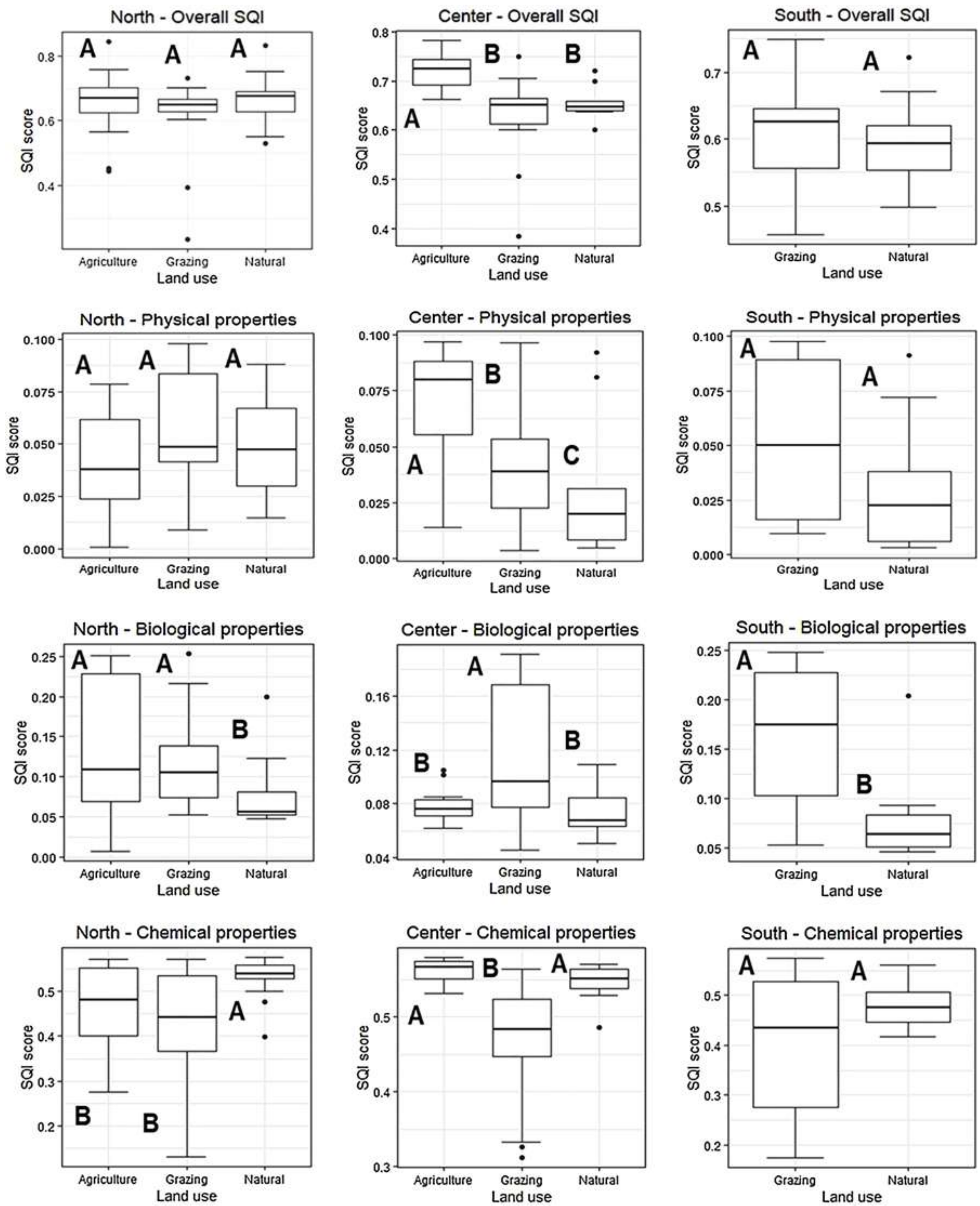

Fig. 5. Scores of soil quality indices (SQIs) and their physical, biological, and chemical components for the three land uses, according to the study area's geographical distribution: north, center and south. Capital letters above the error bars represent significant differences between land uses.

comparing sampling sites. These results demonstrate the high effectiveness, predictability, and reliability of the NIRS model, even in such poor arid soils.

4.1. Soil properties and the soil quality index

Assessment of soil quality was done through an understanding of natural and anthropogenic processes that affect expected soil processes, land use, and management practices, which are represented by a set of multiple different soil properties. This measurement and analysis process of multiple soil properties usually results in high costs and time consumption. The SMAF protocols were used as a guideline for selecting the soil indicators with adjustments that were applied to the physical, biological, and chemical soil properties for developing a statistically modeled integrative SQI. This research sought to evaluate how soil quality and properties are affected under varying LU and management practices. To achieve this goal, data underwent processing and statistical methods, such as logistic transformations and PCA, to define the correct indicators with which to build the appropriate soil quality model. Since this study emphasized soil quality differences in an arid area, the soil indicators were transformed using a scoring function, in which the natural LU was set as a reference when comparing the other

Table 5
Partial least squares-regression (PLS-R) analysis results for the Avdat region. The PLS-R distinguishes between the indicative spectral regions for each soil property. For each soil property in the PLS-R model, the number of latent variables (LV), the coefficient of determination (R^2), the root mean squares error of calibration and cross-validation (RMSEC and RMSECV) of the predicted model, and the ratio of performance to deviation (RPD) are shown. Models with "excellent" (RPD ≥ 2.5 and R^2 ≥ 0.80) and "good" (2 < RPD < 2.5 and R^2 ≥ 0.70) values are marked in bold. Variable importance in projection (VIP) presents the highly significant wavelengths (nm) for each soil property with either excellent or good prediction value.

Soil properties	LV	R^2	RPD	RMSEC	RMSECV	VIP
AWC (%)	2	0.795	1.71	0.243	0.33	
pH	3	0.976	1.58	0.053	0.231	
EC (dS/m)	2	0.958	**3.83**	**4.146**	**5.579**	1363, 1898, 1982
Cl (mg/l)	2	0.960	**3.66**	**50.987**	**70.82**	1836, 1899, 1983
Na (mg/l)	3	0.949	**2.88**	**25.709**	**45.299**	672, 1363, 1896, 1984, 2346
Ca + Mg (mg/l)	2	0.951	**3.22**	**22.351**	**31.644**	1744, 1897, 2003
SAR	2	0.906	**3.19**	**2.204**	**3.243**	671, 1369, 1875, 2056, 2141, 2196, 2270, 2344
NO_3 (mg/kg)	2	0.854	**2.20**	**54.288**	**63.879**	652, 1361, 1420, 1773, 1901, 1974, 2346
P (mg/kg)	2	0.866	**2.19**	**10.864**	**16.352**	450, 597, 1040, 1363, 1415, 1660, 1808, 1884, 1915, 2130, 2254, 2345
SOM (%)	4	0.905	**2.14**	**0.338**	**0.581**	590-739, 853, 1364, 1899, 2014, 2203, 2317
Sand (%)	5	0.882	1.53	3.383	7.053	
Silt (%)	4	0.856	1.74	3.638	5.923	
Clay (%)	2	0.915	1.49	1.409	3.518	
Overall SQI	3	0.903	**2.46**	**0.034**	**0.057**	1434, 1749, 1841, 1901, 1988, 2343

Note: AWC: available water content; EC: electric conductivity; Cl: chlorine; Na: sodium; Ca + Mg: calcium and magnesium; SAR: sodium adsorption ratio; NO3: nitrate; P: phosphorus; K: potassium SOM: soil organic matter; SQI: soil quality index.

two anthropogenic LUs.

The SQI scores showed that in most cases, significant differences were identified. When looking at the mean overall SQI scores, the central agricultural LU was the only one to show significantly higher values. This may imply better soil management of the central agro-ecosystem sampling sites, for which the chemical components (including soil salinity indicators and soil nutrients) had significantly higher values, indicating low saline and well-fertilized soils. This finding is well correlated with higher physical SQI component scores, represented by AWC, indicating well-irrigated fields in the central part, unlike the SQI scores for agriculture in the north that showed an opposite trend (Gupta and Huang, 2014). As expected in an arid area, the AWC levels showed much lower scores in the natural LU in both the central and southern parts, whereas the northern agriculture LU showed relatively similar scores to those of the natural LU. This may indicate poor irrigation in comparison to the central part. For the biological properties represented by NO_3^- and SOM, in all locations, the natural LU displayed significantly lower scores due to low vegetation abundance, fertilizers, and manure input to the soil and livestock activity (Haynes and Naidu, 1998). The high scores of this component for the grazing LU in all geographical units affirm the effects of herding, such as grazing, trampling, urination, and feces, particularly on the levels of pH (Smet and Ward, 2006), soil organic matter (Smet and Ward, 2009), and nitrogen and phosphorus (Perkins and Thomas, 1993).

The results demonstrate that soil quality under different LUs can be measured and distinguished when using an appropriate number of soil indicators. On the one hand, the ability to calculate and produce a reliable and accurate tool for soil quality assessment constitutes the SQI model's significant advantage. On the other hand, the creation of such a tool remains expensive, include extensive soil analyses, and although accurate, it is still explanatory for the point-scale only. Therefore, the correlation to spectral data was performed to reduce the dependence on costly and prolonged soil sampling and laboratory analysis procedures.

4.2. Soil properties and SQI correlations with soil spectroscopy

The results showed that the model managed to predict most soil properties accurately, as well as the SQI (Fig. 6B), when correlated against their respective spectral measurements using PLS-R analysis. In order to evaluate and compare each of the soil properties' prediction performance, the RPD was calculated. The successful prediction performance scores were placed in "excellent" (RPD > 2.5), including EC, Cl, Na, Ca + Mg and SAR, and "good" (2 < RPD < 2.5) categories, including NO_3^-, P, and SOM. The prediction accuracy of each soil property may vary under different locations, and environmental and practical conditions, such as topography, soil composition, time of the year, land and soil management, etc., as well as by sampling point group sizes and numbers and heterogeneous representations of the study area's spatial variability. This can also be seen by the RMSEC and RMSECV values for each soil property. For example, indicators with high RPD scores, such as soil salinity properties (e.g., EC, Cl, Na, Ca + Mg and SAR), also have smaller calibration and cross-validation errors and prediction intervals than other properties, such as NO_3^- and P. In this study, higher R^2 and RPD values are well correlated with lower RMSEC and RMSECV values and present smaller prediction intervals, which confirm the success of the prediction models. RMSEC represents the error of the calibration model, and its error value is always smaller than the one of the RMSECV due to the larger number of observations, which minimizes error sizes (Wise et al., 2006). Trends can be seen in the PLS-R correlation plots in Fig. 6A. For example, as mentioned in the previous section, soil salinity properties showed significant differences in the agricultural LU between the northern and the central parts. Higher values, which correspond to the under-treated fields in the northern part, are distinct from the lower salinity levels in the well-managed fields in the center. This corresponds to the higher SQI scores shown in Fig. 6B. Similarly, SOM concentrations were significantly higher under the agricultural and grazing LUs, whereas in the natural soils, the spectral regression confirmed much lower levels. The same is true for soil nutrients such as NO_3 and P. The prediction of overall SQI (Table 5, Fig. 6B) resulted in "good" performance values ($R^2 = 0.903$, RPD = 2.46, RMSEC = 0.034, RMSECV = 0.057). This was made possible not only by each soil property's contribution to the model but also by the interaction between them all and the spectroscopy data under an integrative index approach.

The PLS-R analysis also generated the recognition of significant sensitivity bands for soil properties. The detection of differences between LUs and sampling sites based on spectral-specific bands can be attributed to chromophores. Chromophores are defined by their physical and chemical interactions with electromagnetic radiation, which affect certain spectral regions, notably in the VIS-NIR (Muller, 1994), although many elements in the soil show sensitivity in the SWIR region as well (Ben Dor et al., 2015). Prevalent molecular bonds, such as C—H, N—H, C—O, C—N, and O—H groups, create different chromophores (Bushong et al., 2015; Fidêncio et al., 2002). Hence, they allow the

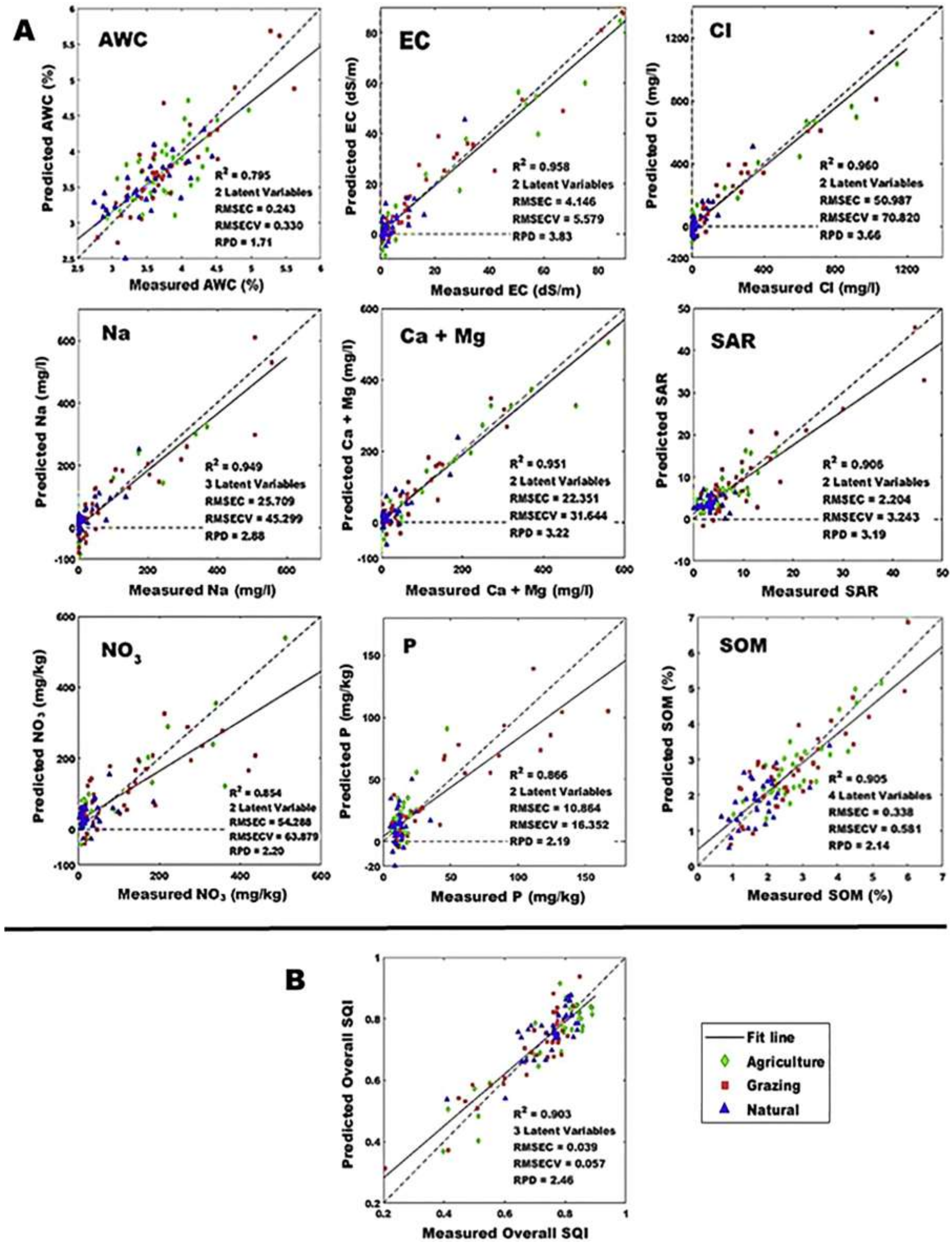

Fig. 6. Partial least squares-regression (PLS-R) correlation scatterplots of predicted cross-validation (CV) values versus soil laboratory analysis values for: (A) several soil properties and (B) the soil quality index (SQI) among the three LUs in the Avdat region. RMSEC: root mean square error of calibration; RMSECV: root mean square error of cross-validation; EC: electric conductivity; Cl: chlorine; Na: sodium; Ca + Mg: calcium and magnesium; SAR: sodium adsorption ratio; NO_3: nitrate; P: phosphorus; SOM: soil organic matter. Each colored shape represents a land-use type: natural ecosystem (blue triangles), agro-pastoral grazing (red squares) and agriculture (green rhombuses).

detection of a variety of soil properties, such as SOM, AWC, EC, pH, and soil texture characteristics (Cécillon et al., 2009; Gholizadeh et al., 2013; Marakkala Manage et al., 2018). The results of the highly significant soil salinity indicators within the 1350–1450 nm, 1830–1990 nm, and 2200–2350 nm spectral ranges are attributed to the presence of hygroscopic water and carbonate, which derives from the predominant sandy-loam soil texture (Table 2) (Ben Dor et al., 2015). Sensitivity bands for the biological properties, including SOM and NO_3, were generated by the model as well, in which SOM peak wavelengths were found in several regions across the VIS-NIR-SWIR. For SOM, the

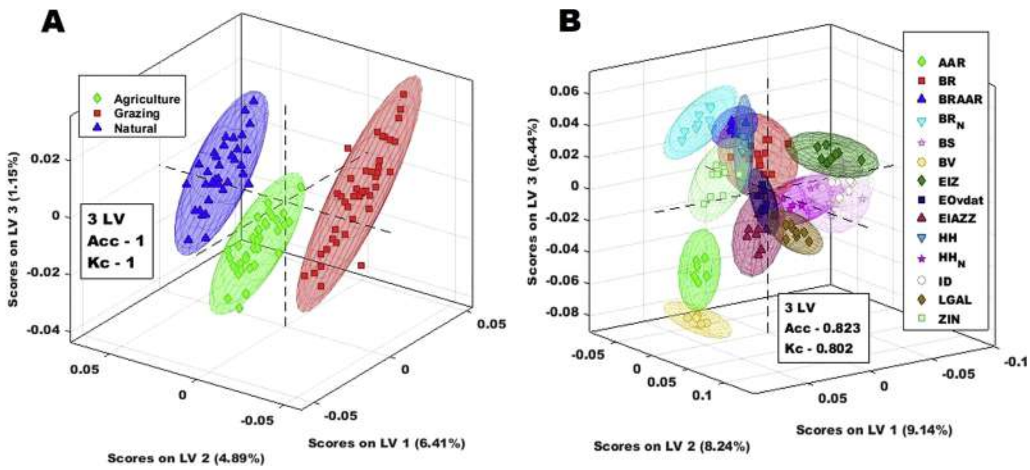

Fig. 7. Partial least squares-discriminant analysis (PLS-DA) classification of initial 2150 bands spectral resolution laboratory spectroscopy for both (A) LUs and (B) sampling sites in the Avdat region. Each figure includes the number of latent variables (LV) used, overall accuracy (Acc), and Kappa coefficient (K_c) values for each model. Colored circles indicate a 95% confidence level. Full names and number of soil samples for all sampling sites are presented in Table 1.

presence of organic matter (i.e., plant tissues, humus, manure, etc.) is connected to the C—H bond and VIS-NIR absorption peaks at the wavelength range of 590–739 nm, and microbial activity and water retained in the soil and in the organic matter itself generated the peaks at 1350–1450 nm and 2200–2350 nm, respectively (Ben-dor, 2017). Although nitrogen is known for its lack of direct universal absorption wavelengths (He et al., 2005), it can be measured by indirect absorption of the soil features mentioned above. The model for NO_3 found several sensitivity bands, notably at 562, 1420, 1901, and 1974 nm, related to water absorbed in the organic compounds, and at 1773 nm, which can be related to free and/or structural iron content (Ben-Dor and Banin, 1995; Rinnan and Rinnan, 2007). The resultant bands for the SQI prediction comprise the most dominant contributors to the model's variability and sensitivity. Hence, the strongest significances are attributed to water absorption, organic matter, and carbonate abundance, with their respective wavelengths previously mentioned. These results strengthen the use of NIRS as a reliable, non-destructive, and time-efficient tool for soil quality analysis. Soil spectroscopy stands out as an adequate and reliable approach for individual soil properties and the multivariate evaluation of SQI. Thus, PLS-R is suitable as a time- and cost-efficient method for analyzing a big dataset of soil samples under a broad set of variables testing soil quality.

4.3. LU and sampling sites' spectral classification

To test the capabilities of the spectral signatures' classification in the model, a partial least squares discriminant-analysis (PLS-DA) was calculated for both different LUs and sampling sites. For the LU-based classifications, both the overall accuracy and the Kappa coefficient had an absolute value of 1. This indicates the success of the model to predict and classify the data accurately. For the sampling site classification (Fig. 7B), the performances were less accurate. Both the overall accuracy and the Kappa coefficient results were significantly lower than those of the LU-based classification, resulting in more significant spectral mixing among groups, possibly due to the smaller sampling size. Hence, it could be concluded that the success of the classification is affected by a set of influencing factors, including the spectral separability and variance between classes, the number of grouping classes, the sample number, the spectral resolution, the noise-induced mistakes, and the modification of raw spectral signatures using PPTs. The PPTs transform and enhance the spectral separability between classes and strengthen the grouping factor within each category, hence, improving the classification accuracy of the model. In this study, the autoscale transformation and GLSW were applied and resulted in the best separation between classes, the smallest CV errors, and the highest classification accuracy.

5. Conclusions

In this study, we aimed to demonstrate the effects of LU activity, represented by human-dominated LUs, on the natural landscape in an arid environment, by evaluating and comparing their soil quality. This goal was achieved by conducting a comparative analysis of both soil laboratory surveys and reflectance spectroscopy of the VIS-NIR-SWIR spectral regions. The ability to differentiate between physical, biological, and chemical soil properties plays a major role in the SQI model in recognizing and characterizing various soil processes in an integrative approach. The transformation scoring functions of soil attributes, as an adjustment tool for SQI, is a key principle that makes the SQI model suitable for monitoring the soil quality differences in soil properties between different LUs. The addition of the spectral dimension into the analysis has proved the effectiveness of NIRS as a comprehensive, non-destructive, and time- and cost-efficient method for monitoring and assessing soil quality and a variety of soil properties based solely on spectral differences. Results back these claims, in which the predicted SQI scores are well correlated with their calculated values (R^2 = 0.903, RPD = 2.46, RMSEC = 0.034, RMSECV = 0.057). Almost all soil properties could be predicted with at least "moderate" performance value, although only those with "good" and "excellent" scores are likely to be used as model prediction accuracy representatives. The implementation of advanced mathematical and statistical methods, such as linear parametric transformations, PCA, PLS-R, and PLS-DA, helps to solve the challenges linked to the multi-dimensional and high-collinearity of some variables in the analysis process. This advantage is reflected in the significant improvement of the results, demonstrating the soil property and SQI prediction accuracy. However, despite its excellent performance, the model is spatially limited to a site-specific point scale. To provide a complete accurate assessment of an entire region's soil quality, upscaling of the spectral resolution would be necessary in future research. This would enable the SQI to be mapped at any given location, which would deepen the understanding of soil functions' spatial trends and improve land management sustainability and conservation in the future.

Conflict of interest

Nothing declared.

Acknowledgments

The project leading to this research was partially funded by the European Union's Horizon 2020 Research and Innovation Programme under grant agreements no. 641762 (Ecopotential).

Appendix A

See Fig. A1.

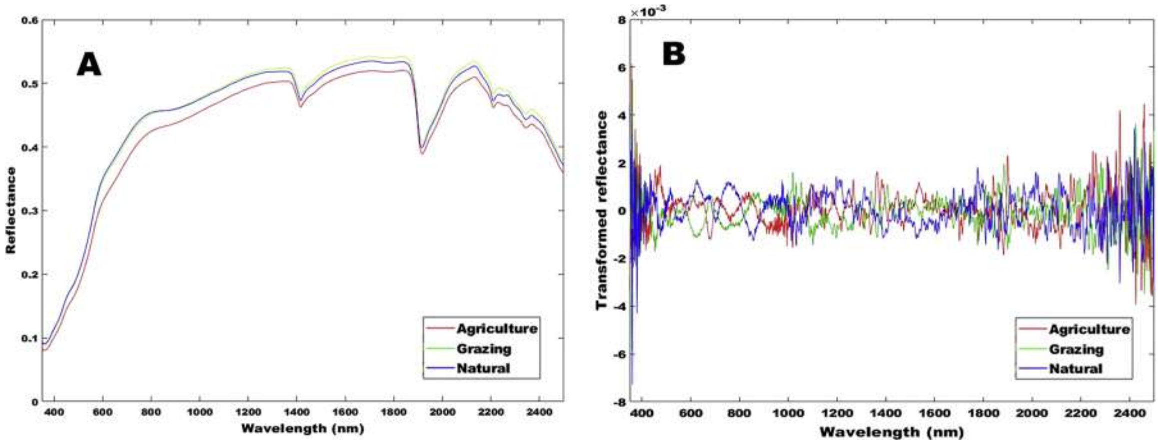

Fig. A1. Mean signatures of soil samples by the three land use types for (A) raw spectral readings, and (B) transformed spectral data using the combination of two preprocessing transformations (PPTs) – (1) autoscale and (2) generalized lest-squares weighting (GLSW).

Appendix B. Supplementary data

Supplementary material related to this article can be found, in the online version, at doi:https://doi.org/10.1016/j.still.2020.104571.

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