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Using Machine-Learning Algorithms to Predict Soil Organic Carbon Content from Combined Remote Sensing Imagery and Laboratory Vis-NIR Spectral Datasets

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Abstract: Understanding spatial and temporal variability in soil organic carbon (SOC) content helps simultaneously assess soil fertility and several parameters that are strongly associated with it, such as structural stability, nutrient cycling, biological activity, and soil aeration. Therefore, it appears necessary to monitor SOC regularly and investigate rapid, non-destructive, and cost-effective approaches for doing so, such as proximal and remote sensing. To increase the accuracy of predictions of SOC content, this study evaluated combining remote sensing time series with laboratory spectral measurements using machine and deep-learning algorithms. Partial least squares (PLS) regression, random forest (RF), and deep neural network (DNN) models were developed using Sentinel-2 (S2) time series of 58 sampling points of bare soil and according to three approaches. In the first approach, only S2 bands were used to calibrate and compare the performance of the models. In the second, S2 indices, Sentinel-1 (S1) indices, and S1 soil moisture were added separately during model calibration to evaluate their effects individually and then together. In the third, we added the laboratory indices incrementally and tested their influence on model accuracy. Using only S2 bands, the DNN model outperformed the PLS and RF models (ratio of performance to the interquartile distance RPIQ = 0.79, 1.36 and 1.67, respectively). Additional information improved performances only for model calibration, with S1 soil moisture yielding the most stable improvement among three iterations. Including equivalent indices of the S2 indices calculated using soil spectra obtained under laboratory conditions improved prediction of SOC, and the use of only two indices achieved good validation performances for the RF and DNN models (mean RPIQ = 2.01 and 1.77, respectively).

Keywords: soil organic carbon; deep learning; Sentinel-2; spectral indices; Sentinel-1; soil moisture; radar indices; visible-near-infrared spectra

1. Introduction

Soil organic carbon (SOC) content is a key parameter that helps assess soil quality. Comprehension of its spatial and temporal dynamics facilitates simultaneously a better assessment of soil fertility and several parameters that are closely associated with it, such as structural stability, nutrient cycling, biological activity, and soil aeration [1–3].

Its regular monitoring has prompted the research community to investigate the reliability of rapid, non-destructive, and cost-effective assessment methods as alternatives to conventional methods.

Soil spectral information is particularly relevant for estimating soil physical–chemical properties, especially organic matter and organic carbon content [4–9]. Different types of proximal, aerial, or satellite sensors have been used, each with different spectral and spatial resolutions [4,7,10,11]. Despite considerable advances in multispectral and hyperspectral remote sensing imagery, their signal-to-noise ratio depends on a variety of parameters not encountered with laboratory spectroscopy [12]. Laboratory soil spectra are acquired under controlled conditions to avoid interfering factors, while remote sensing spectra are influenced by the non-transparent atmosphere and the subpixel composition [13,14], as well as by soil surface roughness, which causes bidirectional effects [7,14,15], and soil moisture [14,16–19]. Given its high spectral resolution, visible and near-infrared (Vis-NIR) spectroscopy is the most accurate method for estimating SOC content, but it provides only point estimates in space [20–26]. Remotely sensed imagery from optical satellites allows for area-based estimates but with lower prediction accuracy [8,27–35]. The performance of the developed models varies according to the spatial scale of the studied area for both laboratory and remotely sensed spectra.

To increase the accuracy of models developed using remote sensing data, in particular multispectral satellite and/or airborne imagery, three main approaches have been developed: (1) Inclusion of spectral indices to consider effects of interference factors [30,33,36–38], especially for several dates in a time series [30,38]; (2) Combination of remotely sensed data with laboratory or field spectra to fuse spectral and spatial soil information [18,35,39–42]; (3) Combination of spectral information from optical images with non-spectral covariates, such as digital elevation models, soil and land use maps, or meteorological and environmental data [43–47]. Other studies have used both synthetic aperture radar (SAR) data and derive predictors (e.g., radar indices, soil moisture) as covariates [48–51] or as a way to select relevant Sentinel-2 dates by estimating the state of the soil surface [38,50].

The increasing availability of spectral data (proximal and remotely sensed), computational power, and interest in data science has favored a transition from linear methods to machine-learning algorithms in soil science [52,53] and, more recently, to deep-learning techniques [54]. Machine-learning algorithms, such as support vector machine (SVM) regression, random forest (RF), and cubist regression (CR), have shown their ability to analyze non-linear relationships between spectral information and SOC content when compared to multiple linear regression and partial least squares (PLS) regression [55–58]. Furthermore, studies of neural networks have found them to perform significantly better than other techniques. For example, Haghi et al. [58] and Ng et al. [59] found that convolutional neural networks (CNN) outperform CR, SVM, and PLS regression models when using laboratory reflectance spectra. Similarly, artificial neural networks and deep neural networks (DNN) predicted SOC content well using laboratory spectra [60,61] but, to our knowledge, have rarely been tested using reflectance spectra from satellite images. Moreover, previous studies used either a single-date image (e.g., [27,29,30,58]) or a temporal mosaic that produced a single aggregated reflectance spectrum over a time series (e.g., [25,28,35]), but did not use multiple dates to represent changes in the soil surface in the models.

The present study aimed to increase the accuracy of SOC content predictions using two complementary mechanisms: (i) Enriching the information considered by combining remote sensing time series and laboratory spectral measurements; (ii) Improving model accuracy using machine-learning algorithms. To this end, we used Sentinel-2 remote sensing data of bare soil and combined them with Sentinel-1 SAR-derived data and indices derived from Vis-NIR laboratory spectra to predict SOC content in an agricultural study area. We also compared the performance of PLS regression, RF, and DNN models in predicting SOC content.

2. Materials and Methods

2.1. Study Area and Soil Sampling

The study area is an agricultural land covering ca. 1.5 km^2 in the northwestern section (48°0′40″N, 2°50′40″W) of the Naizin watershed (western France). The fields studied were located on both sides of a small tributary of the Coët-Dan stream with a moderate slope (<5%). Fields in the northern part have the steepest slopes, with slopes of between 3% and 5%, while those in the southern part are less than 2%. The climate is temperate, with mean annual rainfall of ca. 909 mm. Agriculture is mainly intensive, with cereals, maize, and grassland as the main land uses in crop rotations. The soils are developed on a silty substrate derived from weathered schists and Quaternary aeolian deposits. The dominant soil types are Luvic Cambisols and Haplic Albeluvisols of silty texture [62–64].

We sampled 83 points within 22 fields in October 2020. These sampling points were selected using a 100 m triangular grid, except in small fields, in which points were selected randomly (Figure 1). Within 5 m of each point, 5 subsamples of soil were collected randomly from the top 5 cm and then pooled. The samples were air-dried, sieved to 2 mm, and divided in half by sample quartering: one half was sent to the national INRAE soil analysis laboratory (LAS Arras, France) for soil analysis, while the other was used to measure reflectance spectra under laboratory conditions. The SOC content was measured via dry combustion according to certified method NF ISO 10694 [65].
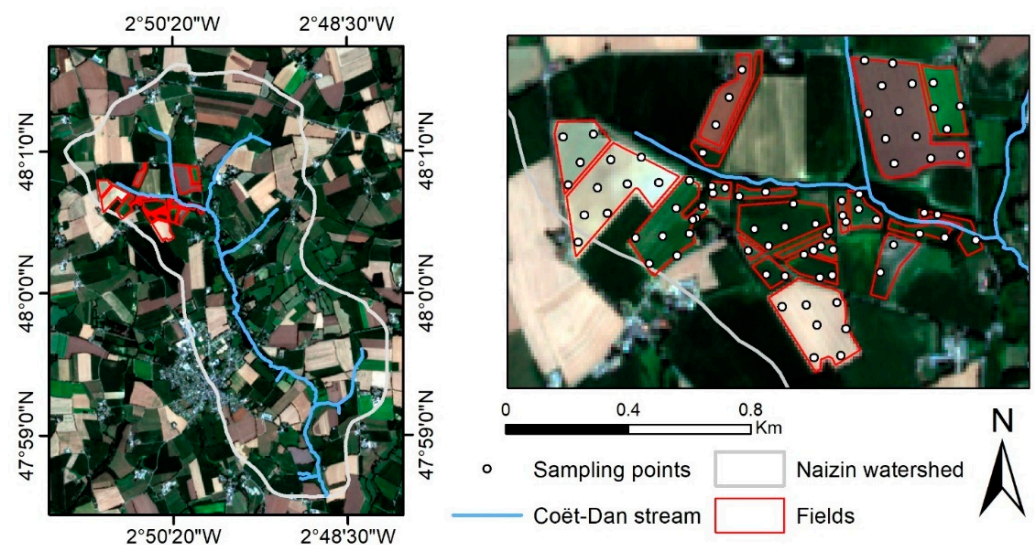

Figure 1. Maps of the study area in Naizin watershed and its sampling points.

2.2. Laboratory Reflectance Measurements

Soil spectra were measured under laboratory conditions. The 2 mm sieved soil samples were oven-dried at 40 °C for 24 h. Their spectra were then measured using a full range spectroradiometer (ASD FieldSpec® 3, Malvern Panalytical Ltd., London, UK). For each sample, the instrument was calibrated using the white reference standard (Spectralon®, North Sutton, NH, USA) before scanning the soil four times at different positions with the contact probe. Since the spectrometer is equipped with three different detectors [66], the spectra were splice-corrected using ViewSpecPro software to eliminate signal jumps that can occur when changing detector ranges [67]. The mean of the four reflectance spectra in the 400–2450 nm range was used to maximize the signal-to-noise ratio.

2.3. Sentinel-1 and Sentinel-2 Data Pre-Processing

A time series of 80 Sentinel-2 Level-2A images corresponding to our study area (110 × 110 km tile: T30SNE) and acquired from September 2020 to August 2021 were downloaded from the Theia website "https://www.theia-land.fr/ (accessed on 15 October 2021)". These data are atmospherically corrected using the MAJA processing chain [68] and correspond to ortho-rectified surface reflectance. They cover 10 bands ranging from visible to near-infrared wavelengths and are provided with a mask for clouds and their shadows [69].

After applying the cloud mask, we selected the 26 images with low cloud cover (≤5%) for our study area. We then resampled bands with 20 m spatial resolution to 10 m using the nearest-neighbor assignment method. Following analysis of NDVI profiles, the reflectance of bare soil was extracted using an NDVI threshold [29,70,71]. Pixels with an NDVI <0.25 were considered as bare soils. Only 58 of the 83 sampling points were bare soils on at least one date during the 2020–2021 agricultural season.

The dual-satellite constellation of Sentinel-1A and Sentinel-1B was launched in April 2014 and April 2016, respectively. It provides C-band (frequency = 5.4 GHz) SAR images with a revisit time of 6 days in dual-polarization VV (vertical-vertical) and VH (vertical-horizontal) modes. In this study, we used Level-1 ground-range-detected products acquired from September 2020 to August 2021. Sentinel-1 images were downloaded using the Google Earth Engine application, which provides radar signal images processed for thermal noise removal, radiometric calibration, terrain correction, and speckle filtering.

2.4. Sentinel-1 Soil Moisture and Indices Retrieval

From the downloaded Sentinel-1 time series we extracted the radar signal corresponding to bare soils and calculated three radar indices (S1-indices) from its two polarizations (Table 1). For each sampling point, the radar signal was averaged over its corresponding polygon of Thiessen, in the linear scale, then converted to the logarithmic scale and used for S1-indices calculation. If the Sentinel-1 image was acquired on the same date as a Sentinel-2 image, we automatically used it. If not, we calculated the mean radar signal of the two closest dates before and after the Sentinel-2 visit, with an interval not exceeding two days. If only one date was available in the two-day interval, either before or after the Sentinel-2 visit, we used it. In addition, we used estimates of volumetric soil moisture (%) derived from the Sentinel-1 time series (S1-soil moisture) using the approach of El Hajj et al. [72] and validated for our study area by Zayani et al. [73].

Table 1. Equations of the Sentinel-1 indices used.

Abbreviation	Index	Equation	Reference
R1	Radar cross ratio	$\frac{VH}{VV}$	[74]
R2	Radar ratio 2	$\frac{VH + VV}{VV}$	[74]
D	Radar difference	$VH - VV$	[75]

VV: vertical–vertical polarization, *VH*: vertical–horizontal polarization.

2.5. Retrieval and Analysis of Spectral Indices

In addition to the spectral bands, spectral indices have been developed and used to analyze remote sensing images. These indices are calculated using common equations and enhance some spectral features by minimizing effects of illumination and reducing noise [76,77]. In this study, we used the bare-soil reflectance extracted from the Sentinel-2 images to calculate 40 spectral indices (Appendix A). Based on their application in previous studies, these indices can be grouped into four categories: vegetation, soil, geology, and water. To identify the indices that improved detection of soil variability in space and time, we performed multiple factor analysis (MFA) of the time series of indices for the 58 points of bare soil. This multivariate method, MFA [78] is based on principal component analysis (PCA) and used to summarize data described by several sets of variables organized into

groups. Variables of the same group are normalized with a weight equal to the inverse of the first eigenvalue of the PCA, and each variable of the group has its own weight. In our study, each time series of indices was considered as a group. We selected twelve indices that contributed differently to the first two dimensions of the MFA in order to use them to calibrate the models (S2-indices) (Table 2). We then calculated the same 12 indices using the soil spectra measured in the laboratory and the central wavelengths of the Sentinel-2 bands (Lab-indices). To decrease the number of indices potentially included in the prediction models, we selected optimal indices that had the highest Pearson correlation coefficients with SOC content.

Table 2. Equations of the Sentinel-2 spectral indices selected based on multiple factor analysis and equations of the corresponding laboratory spectral indices. Subscripts in the latter equations indicate the central wavelengths of the Sentinel-2 bands.

Ab.	Index	Equation for Sentinel-2 Indices	Equation for Laboratory Spectral Indices	Ref.
		Vegetation indices		
AFRI21	Aerosol free vegetation index 2.1	$\frac{B8A - 0.5 \times B12}{B8A + 0.5 \times B12}$	$\frac{R_{865} - 0.5 \times R_{2202}}{R_{865} + 0.5 \times R_{2202}}$	[79]
ARVI2	Atmospherically resistant vegetation index2	$-0.18 + 1.17 \times \left(\frac{B8 - B4}{B8 + B4} \right)$	$-0.18 + 1.17 \times \left(\frac{R_{832} - R_{665}}{R_{832} + R_{665}} \right)$	[80]
GVMI	Global vegetation moisture index	$\frac{(B8 + 0.1) - (B12 + 0.02)}{(B8 + 0.1) + (B12 + 0.02)}$	$\frac{(R_{832} + 0.1) - (R_{2202} + 0.02)}{(R_{832} + 0.1) + (R_{2202} + 0.02)}$	[81]
Maccioni	Maccioni vegetation index	$\frac{B7 - B5}{B7 - B4}$	$\frac{R_{783} - R_{704}}{R_{783} + R_{704}}$	[82]
NBR	Normalized burn ratio	$\frac{B8 - B12}{B8 + B12}$	$\frac{R_{832} - R_{2202}}{R_{832} + R_{2202}}$	[83]
NBR2	Normalized burned Ratio 2	$\frac{B11 - B12}{B11 + B12}$	$\frac{R_{1614} - R_{2202}}{R_{1614} + R_{2202}}$	[84,85]
NDVI	Normalized difference vegetation index	$\frac{B8 - B4}{B8 + B4}$	$\frac{R_{832} - R_{665}}{R_{832} + R_{665}}$	[70]
SIWSI	Shortwave infrared water stress index	$\frac{B8A - B11}{B8A + B11}$	$\frac{R_{865} - R_{1614}}{R_{865} + R_{1614}}$	[86]
TSAVI	Soil-adjusted vegetation index	$\frac{1.22 \times (B8 - 1.22 \times B4 - 0.03)}{1.22 \times B8 + B4 - 1.22 \times 0.03 + 0.08 \times (1 + 1.22^2)}$	$\frac{1.22 \times (R_{832} - 1.22 \times R_{665} - 0.03)}{1.22 \times R_{832} + BR_{665} - 1.22 \times 0.03 + 0.08 \times (1 + 1.22^2)}$	[87]
		Soil indices		
BI	Brightness index	$\sqrt{\frac{B2^2 + B3^2 + B4^2}{3}}$	$\sqrt{\frac{R_{492}^2 + R_{560}^2 + R_{665}^2}{3}}$	[88,89]
BSI	Bare soil index	$\frac{(B12 - B4) - (B8 - B2)}{(B12 - B4) + (B8 - B2)}$	$\frac{(R_{2202} - R_{665}) - (R_{832} - R_{492})}{(R_{2202} - R_{665}) + (R_{832} - R_{492})}$	[90]
		Water indices		
NDMI	Normalized difference moisture index	$\frac{B8 - B11}{B8 + B11}$	$\frac{R_{832} - R_{1614}}{R_{832} + R_{1614}}$	[91]

Ab.: Abbreviation, Ref.: Reference.

2.6. Prediction Models and Accuracy Assessment

Models were calibrated using three approaches (Figure 2). In the first, only S2 bands (a) were used for model calibration to compare the performance of PLS regression, RF, and the DNN. Based on the results of approach 1, only the two algorithms with the best prediction performance in cross-validation were retained for use in the following two approaches. In the second approach, S2-indices (a + b), S1-indices (a + c), and S1-soil moisture (a + d) were used separately during calibration to assess their individual effects and then used together (a + e). In the third approach, the Lab-indices were added incrementally in the order of decreasing correlation with SOC content (NBR2, NDVI, ARVI2, Maccioni, and TSAVI) to assess their effects on model accuracy. To group all available Sentinel-2 data with bare soil, we constructed a table with 512 rows, which corresponded to "point × date" individuals for the 58 sampling points that had bare soil (range: 1–18 dates). We then randomly split the data into calibration (70%) and validation (30%) datasets. To test the robustness of our approaches, we performed three iterations of each.
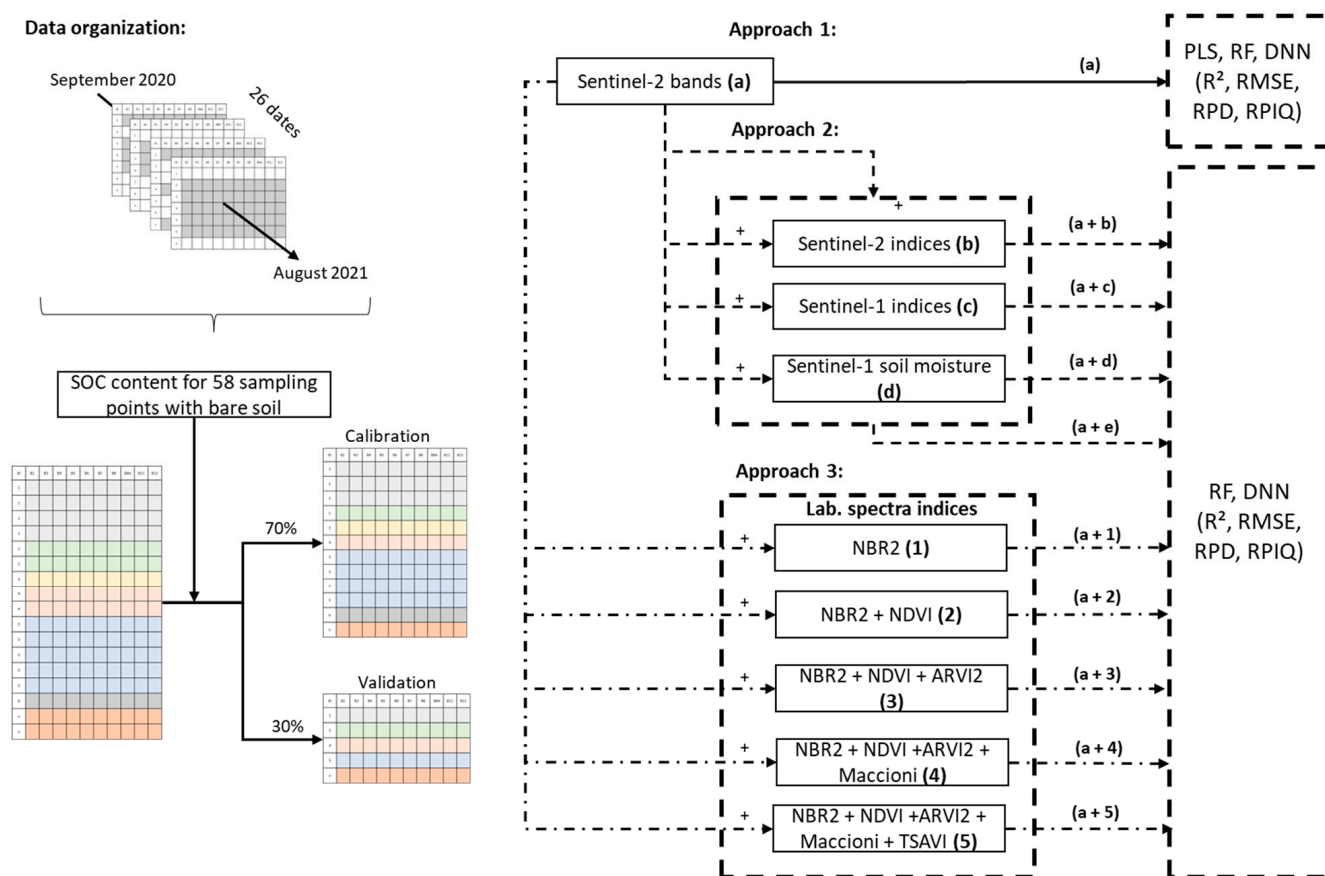
Figure 2. Flowchart of data organization and developed approach for combining Sentinel-2 bands with Sentinel-2 indices, Sentinel-1 indices, Sentinel-1 soil moisture, and laboratory spectral indices. Colors in tables of the data indicate the available dates for each soil sample. See Table 2 for definitions of the spectral indices. PLS: partial least squares, RF: random forest, DNN: Deep neural network, R^2: coefficient of determination, RMSE: root mean square error, RPD: ratio of performance to deviation, RPIQ: ratio of performance to interquartile distance.

2.6.1. Partial Least Squares Regression

PLS regression is the most common linear regression used to predict soil properties. Developed by Wold [92], it maximizes the variance of spectral variables by reducing the original dimension of the spectra into latent variables. It extracts useful components that are strongly correlated with the dependent variables and overcomes problems of multicollinearity between spectral variables [93]. PLS regression performs better than other linear regression methods because of the stability of its latent variables. However, it is sensitive to outliers in the dataset [94] and forces predictions towards the center of the calibration dataset. Thus, for samples with high leverage, prediction uncertainty increases [95]. Non-linear iterative PLS (NIPALS) and statistically inspired modified PLS are the two most common optimization algorithms of PLS regression. In this study, we used the NIPALS algorithm implemented in the scikit-learn 1.0.2 package (Python 3.7.4), which aims to linearize models that have non-linear parameters [92,96]. The optimal number of components was selected using both the coefficient of determination (R^2) and the RMSE of a 5-fold cross-validation (RMSECV) and relying on the grid search method (Table A2 in Appendix B). This method allows models parameters to be adjusted by searching a grid of all possible combinations and evaluating them using cross-validation (Figure 3) [97,98].
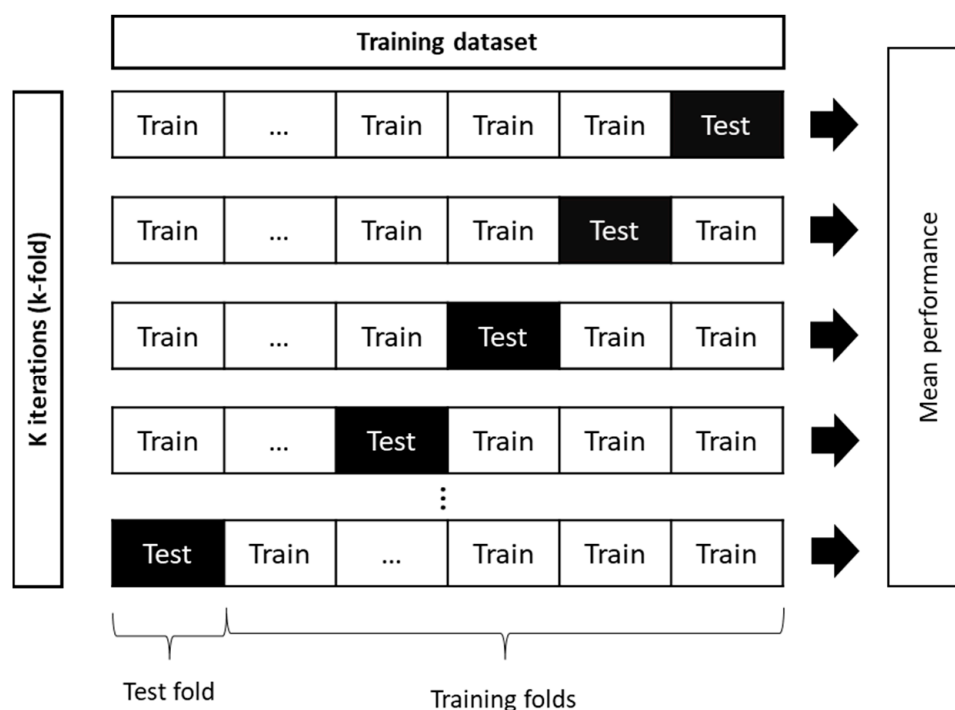
Figure 3. Schematic diagram of k-fold cross validation principle (adapted from Phung and Rhee (2019) [99]).

2.6.2. Random Forest

The RF is an ensemble of randomized classification and regression trees that generates multiple decision trees from a randomly selected subset of training samples and uses averaging to increase prediction performance and control overfitting [100]. Many individual trees are trained from bootstrapped subsets of the data, which results in individual learning algorithms being run (Figure 4a). The final prediction equals the mean of these suboptimal trees. The number of trees (n_estimators), the maximum depth of the trees (max_depth), and the number of samples used in each node are user-defined parameters that influence the prediction performance and model efficiency. For example, if the n_estimators value is too large, it will affect the model computation; if it is too small, the model error will not stabilize [101,102]. A higher number of samples used in each node helps to prevent overfitting by avoiding more specific trees [102]. Like other machine-learning algorithms, RF is increasingly used to predict soil properties. It has been shown to increase prediction performance due to its excellent non-linear learning ability and flexibility. In this study, optimal hyperparameters (max_features and max_depth corresponding to the number of features to consider when looking for the best split and the maximum depth of the tree, respectively) were adjusted based on the RMSECV using the "RandomizedSearchCV" and "RandomForestRegressor" functions implemented in the scikit-learn 1.0.2 package (Python 3.7.4) (Tables A2 and A5 in Appendix B). Randomized search is an alternative method to the grid search method and it performs a random search for hyperparameters within a predefined grid. A fixed number of iterations is performed, and at each iteration the algorithm selects a combination of hyperparameters, tunes the model, and evaluates its performance using RMSECV [97]. The number of trees was fixed at 500 and the number of iterations at 100 for all RF models.
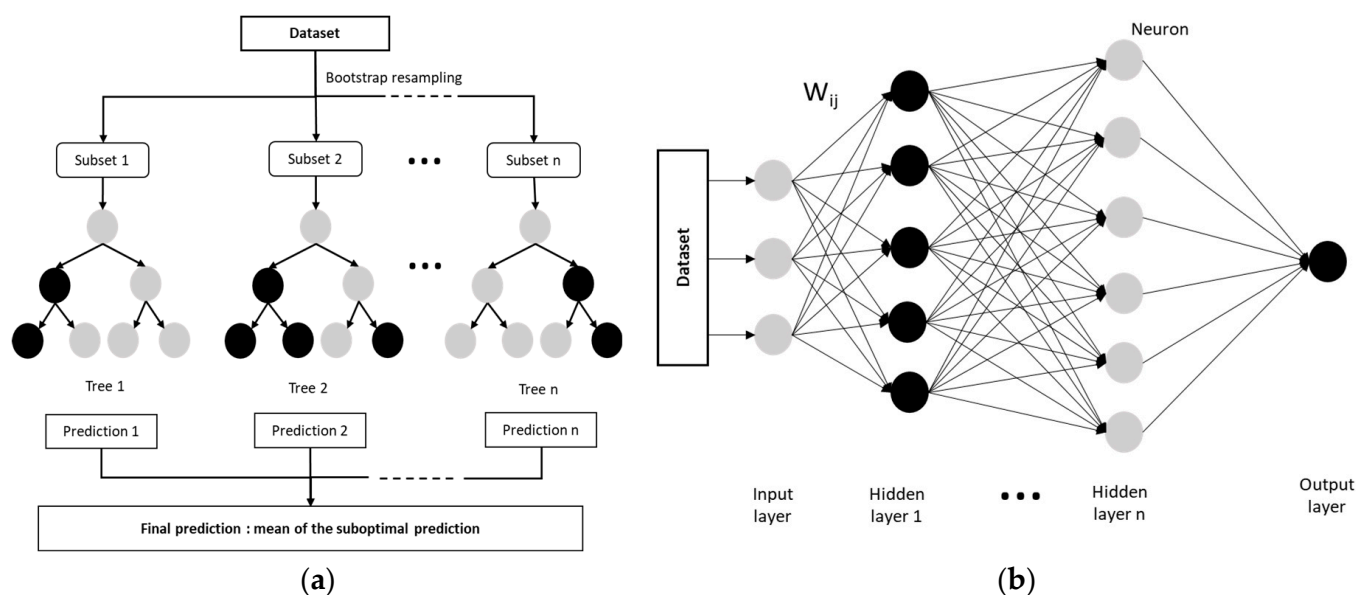
Figure 4. Schematic diagram: (**a**) The Random Forest model structure (adapted from Song et al. (2022) [101]); (**b**) The DNN model architecture (adapted from Liu et al. (2017) [103]).

2.6.3. Deep Neural Networks

Neural networks consist of layers of artificial neurons (also called "perceptrons" or "nodes") that include an input layer, one or more hidden layers, and an output layer. Each node is connected to another and has an associated weight and threshold. It, thus, combines inputs with a set of coefficients that either amplify or dampen that input. An activation function then determines whether and to what extent that signal should progress further through the network to influence the result. Depending on the nature of the problem studied, neural network architectures can be classified by the number and type of layers used, and the number of nodes, or simply as supervised vs. unsupervised learning networks [103,104]. Among the architectures used to predict soil properties [59,105,106], we used a DNN, which has at least two fully connected hidden layers between the input and output layers and provides linear and non-linear relationships between the response variable and a set of predictor variables (Figure 4b) [103]. It was better suited to our case study than a CNN, which is more adapted to data with spatial structure and most commonly used in remote sensing [107]. Thus, the abundant cloud cover over our study area led to a loss of spatial and temporal information. The rectified linear unit (ReLU) activation function was used to establish relationships between input and output neurons in each hidden layer. The optimal number of hidden layers and neurons in each layer was selected based on the RSME using the "tuner.search" framework implemented in the *keras_tuner 1.1.3* package (Python 3.8.16) (Tables A2 and A5 in Appendix B), which is a scalable hyperparameter optimization framework. It is based on Bayesian optimization, Hyperband, and random search algorithms [108]. The random search strategy was used in our case. It consists of a random selection of hyperparameter combinations according to a defined number of iterations, during which the model is trained for a certain number of epochs. As a result, the algorithm returns the best hyperparameters, corresponding to the combination that gave the best performance [97,108]. In our case, the maximum number of iterations was set to 50 (max_trials = 50), the learning rate to 0.01, and the number of epochs to 50.

2.6.4. Model Accuracy

The prediction performance of models was evaluated using R^2, RMSE, the ratio of performance to deviation (RPD), and the ratio of performance to the interquartile distance (RPIQ) developed by Bellon-Maurel et al. [86]. Higher R^2 and lower RMSE indicate a

higher model prediction accuracy. As suggested by Chang et al. [109], predictions of soil property models were considered poor for RPD < 1.4, moderate for 1.4 < RPD < 2, and accurate for RPD > 2. Similarly, Nawar and Mouazen [110] considered model predictions very poor for RPIQ < 1.4, fair for 1.4 < RPIQ < 1.7, good for 1.7 < RPIQ < 2, very good for 2 < RPIQ < 2.5, and excellent for RPIQ > 2.5. The formulas for the performance parameters are as follows:

$$R^2 = \frac{\sum_{i=1}^{n} (\hat{y}_i - \overline{y})^2}{\sum_{i=1}^{n} (y_i - \overline{y})^2},$$

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n} (\hat{y}_i - y_i)^2}{n}},$$

$$RPD = \frac{STD}{RMSE},$$

$$RPIQ = \frac{Q_3 - Q_1}{RMSE}$$

where y_i indicates the measured value of SOC content of the ith sample, $\hat{y}_i$ the predicted value of SOC content of the ith sample, $\overline{y}$ the average value of measured SOC content, n the number of samples, (i = 1, 2, 3, . . ., n), and $Q_3 - Q_1$ indicates the interquartile distance. Q_3 is the value below which we find 75% of the samples and Q_1 is the value below which we find 25% of the samples.

3. Results

3.1. Data Description and Analysis

3.1.1. Descriptive Statistics of Measured SOC Content

The measured SOC contents of the 58 sampling points that were in bare soil, ranged from 15.2–49.4 g·kg^{-1}, with a mean of 22.3 g·kg^{-1} (Table 3). They lay within the range of SOC content usually observed in the Naizin watershed and were consistent with those measured in a previous study [111]. The descriptive statistics of the calibration and validation datasets generated for the three iterations using the S2 time series are presented in Table 4.

Table 3. Descriptive statistics of soil organic carbon (g·kg^{-1}) content measured at the 58 sampling points that were in bare soil in the study area in 2020.

n	Mean	St. Dev.	Median	Min	Max	Skewness
58	22.3	3.6	21.9	15.2	49.4	3.7

n: Number of soil samples, St. dev.: Standard deviation.

Table 4. Descriptive statistics of soil organic carbon content of the calibration and validation datasets generated for the three iterations.

It.	Dataset	n	Mean	St. Dev.	Median	Min	Max	Skewness
1	Cal	358	22.2	3.5	21.9	15.2	49.4	3.4
	Val	154	22.3	3.9	21.9	17.1	49.4	4.2
2	Cal	359	22.3	3.5	22.0	15.2	49.4	3.6
	Val	153	22.2	4.0	21.8	17.1	49.4	3.8
3	Cal	358	22.5	4.0	22.0	15.2	49.4	3.8
	Val	154	21.9	2.5	21.8	15.2	30.1	0.4

It.: Iteration, Cal: Calibration, Val: Validation, n: Number of individuals, St. Dev.: Standard deviation.

3.1.2. Sentinel-2 and Laboratory Spectral and Sentinel-1 Soil Moisture Information Analysis

The mean reflectance of soil samples was lower for Sentinel-2 spectra than for laboratory spectra (Figure 5a). Some mean S2-indices were lower than mean Lab-indices, while others were higher or nearly the same (Figure 5b). As expected, the former also varied more, since surface conditions, especially soil moisture, varied among sampling points and dates. Some S2-indices (e.g., NBR, BSI) were more sensitive (i.e., variable) than the others. The same was true for Lab-indices, although this variability seemed to be non-significant.
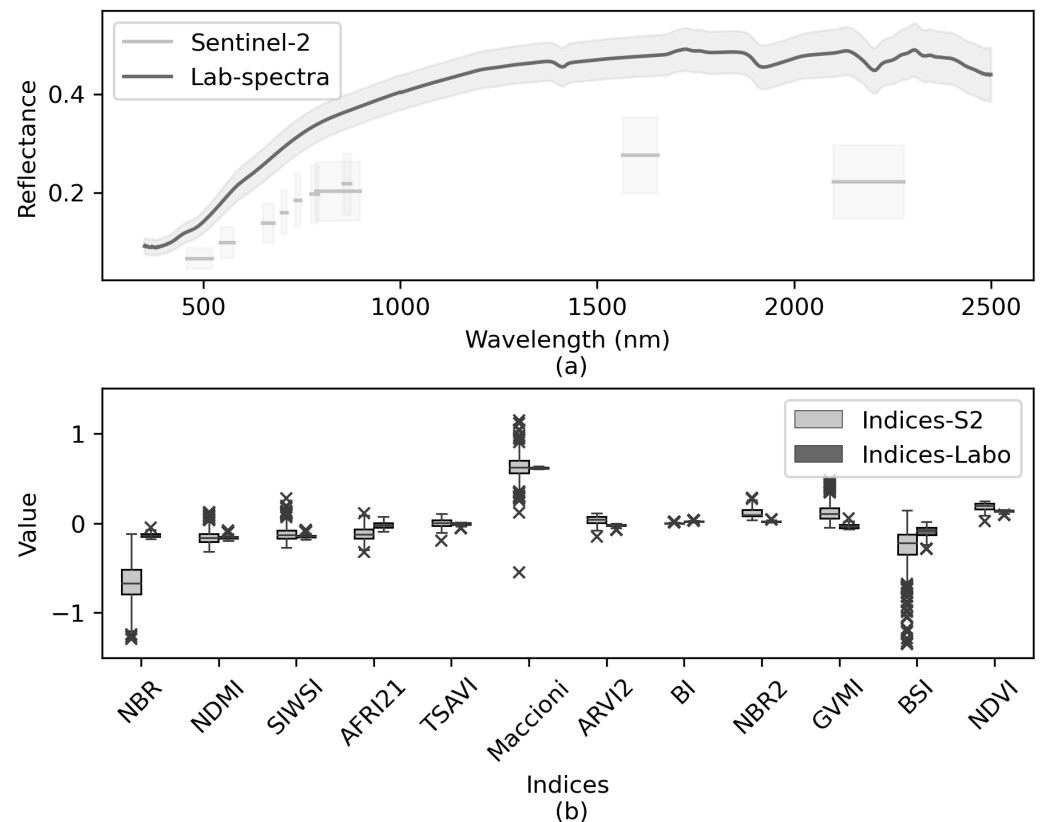

Figure 5. Sentinel-2 vs. laboratory spectral information for the 58 soil samples: (**a**) Mean ± 1 standard deviation of spectra; (**b**) Boxplots of the spectral indices calculated. Whiskers indicate 1.5 times the interquartile range. See Table 2 for definitions of the spectral indices.

The S2-indices explained more than 51% of total inertia on the first two dimensions of the MFA (Figure 6). Most S2-indices contributed to approximately the same degree (>0.75) to dimension 1 but contributed to varying degrees (0.10–0.75) to dimension 2. Indices BSI and GVMI contributed the least to dimension 1 and among the most to dimension 2.

Most correlations between the Lab-indices and SOC content were significant at $p < 0.01$ and had absolute values greater than 0.40 (Table 5). Weaker correlations between the Lab-indices and SOC content (r = 0.20–0.30) were significant only at $p < 0.05$. Indices with r > 0.70 with SOC content were calculated using wavelengths of 665–832 nm, except for NBR2, which used wavelengths of 1614–2202 nm.
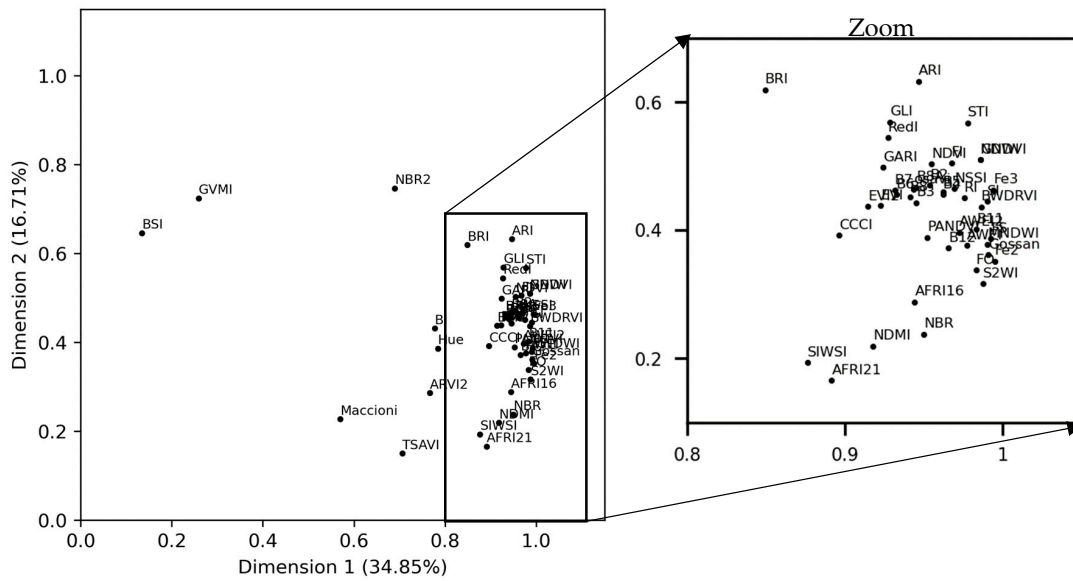
Figure 6. The first factorial plane of the multiple factor analysis (MFA), showing the correlation of the Sentinel-2 indices with the MFA dimensions with a zoom on the condensed part. See Table 2 for definitions of the spectral indices.

Table 5. Pearson correlation coefficients (r) between soil organic carbon (SOC) content and laboratory spectral indices, and their statistical significance. See Table 2 for definitions of the spectral indices.

Index	r
NBR2	0.85 ***
NDVI	0.81 ***
ARVI2	0.81 ***
Maccioni	0.80 ***
TSAVI	0.79 ***
BI	-0.46 ***
GVMI	0.41 ***
NBR	0.26 *
BSI	0.22 *
NDMI	-0.16 ns
AFRI21	-0.20 ns
SIWSI	-0.05 ns

Significance: ns, non-significant; *, $p < 0.05$; ***, $p < 0.001$.

S1-soil moisture varied more than the S1-indices (Figure 7). The mean S1-soil moisture varied from 9.8% to 36.5%, with standard deviations of 0.8–6.8% that were lowest on the dates with the highest soil moisture ($\geq$30%).
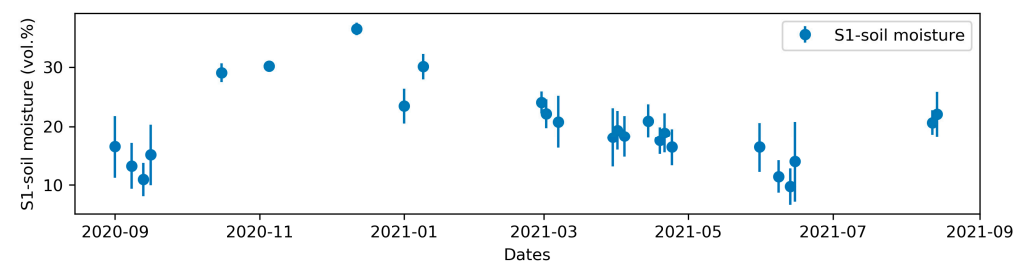

Figure 7. Mean and standard deviation (error bars) of Sentinel-1 soil moisture for bare soils on the 26 dates used during the 2020–2021 crop year.

3.2. Model Performance and Comparison

3.2.1. Sentinel-2 Bands Prediction Performance

The results of the validation of the SOC content models using only the Sentinel-2 bands varied among the algorithms (Figure 8, Table A3 in Appendix B) but were relatively stable among the three iterations, with RMSEP equal to 3.57 ($\pm$0.79), 3.51 ($\pm$0.45), 2.33 ($\pm$0.1), for PLS, RF, and DNN, respectively. However, according to R^2, the third iteration always produce results of poor quality. Based on the RPD, only models calibrated using DNN performed moderately well in predicting SOC content (1.47 ($\pm$0.26)). But, based on the RPIQ, SOC predictions were very poor for the three algorithms (0.93 ($\pm$0.18), 0.90 ($\pm$0.11), and 1.31 ($\pm$0.08)).
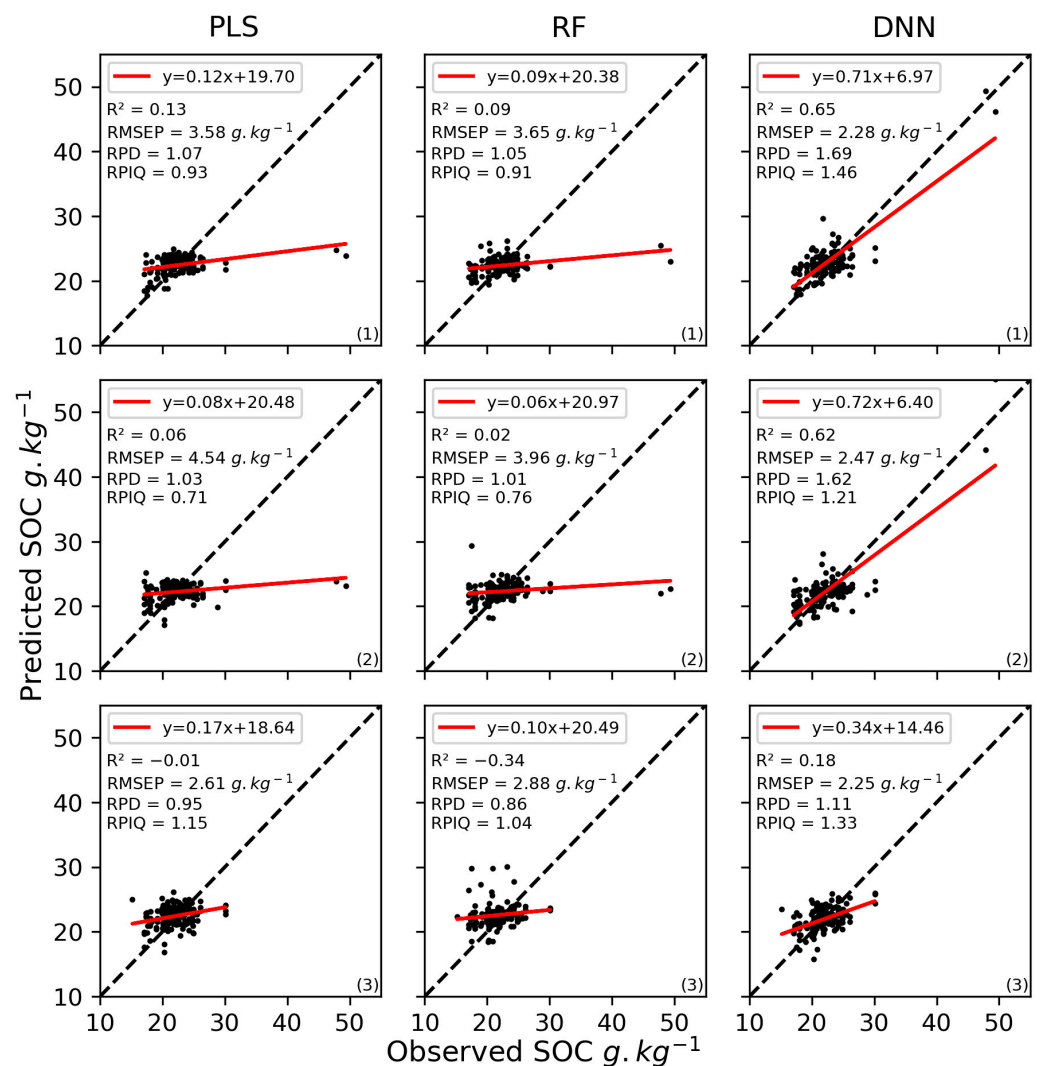
Figure 8. Scatterplots of measured vs. predicted soil organic carbon (SOC) content for the validation dataset using Sentinel-2 bands and the partial least squares (PLS), random forest (RF), or deep neural network (DNN) algorithms for the three iterations ((1), (2), and (3)). R^2: coefficient of determination, RMSEP: root mean square error of prediction, RPD: ratio of performance to deviation, RPIQ: ratio of performance to the interquartile distance.

3.2.2. Prediction Performance of Sentinel-2 Bands Combined with Sentinel-2 and Sentinel-1 Indices and Sentinel-1 Soil Moisture

Including the S1- and S2-indices and S1-soil moisture along with the Sentinel-2 bands in the models influenced calibration performance more than validation and the DNN algorithm performance more than the RF algorithm (Figure 9, Table A4 (Appendix B)). Using

the DNN, the combination of S2-indices, S1-indices, and S2-indices + S1-indices + S1-soil moisture with Sentinel-2 bands increased the calibration performance the most (mean RPIQ = 2.59 ($\pm$1.30), 2.53 ($\pm$1.50), and 2.89 ($\pm$2.16), respectively), but this result was not stable among the three iterations. Model calibration performance was most stable when S1-soil moisture was included for DNN and RF (mean RPIQ = 2.17 ($\pm$0.2) and 1.48 ($\pm$0.08), respectively), but doing so had no strong effect on model validation performance. Thus, for all calibrated models, the RPIQ for model validation was always lower than the RPIQ threshold 1.7 considered for accurate predictions. Based on the mean RPD values, only the DNN model calibrated using S2 bands + S1-soil moisture showed a moderate validation performance of SOC prediction (mean RPD = 1.42 ($\pm$0.31)), but no improvement was observed compared to using only S2 bands (mean RPD = 1.47 ($\pm$0.32)). Mean RMSEP values ranged from 3.34 ($\pm$0.46) to 3.59 ($\pm$0.55) for RF and from 2.33 ($\pm$0.12) to 2.95 ($\pm$0.34) for DNN.

a: Bands
a+b: Bands + Sentinel-2 indices
a+c: Bands + Sentinel-1 indices
a+d: Bands + Soil moisture
a+e: Bands + Sentinel-2 indices + Sentinel-1 indices + Sentinel-1 soil moisture

Figure 9. Mean performance of the three iterations during model calibration and validation using the random forest (RF) and deep neural network (DNN) algorithms when using Sentinel-2 indices, Sentinel-1 indices, and Sentinel-1 soil moisture: (**a**) Ratio of performance to the interquartile (RPIQ); (**b**) Root mean square error (RMSE); (**c**) Ratio of performance to deviation (RPD). Error bars indicate 1 standard deviation. Horizontal red lines indicate performance thresholds (see Section 2.6.4).

3.2.3. Prediction Performance of Sentinel-2 Bands Combined with Laboratory Spectral Indices

Combining laboratory spectral indices with the Sentinel-2 bands to calibrate models to predict SOC content influenced model performance strongly (Figure 10, Table A6 (Appendix B)). For both the RF and DNN algorithms, the validation criteria with mean RPIQ > 1.7 were obtained when including at least the two indices most correlated with SOC content (i.e., NBR2 and NDVI). However, doing so generated high variability in validation performance for the RF models (i.e., standard deviations of RPIQ of 1.13–2.10), while the validation performance of the DNN models remained relatively stable (mean RPIQ of 1.84 ($\pm$0.21) to 3.07 ($\pm$0.72)).

a: Bands
a+1: Bands + NBR2
a+2: Bands + NBR2 + NDVI

a+3: Bands + NBR2 + NDVI + ARVI2
a+4: Bands + NBR2 + NDVI + ARVI2 + Maccioni
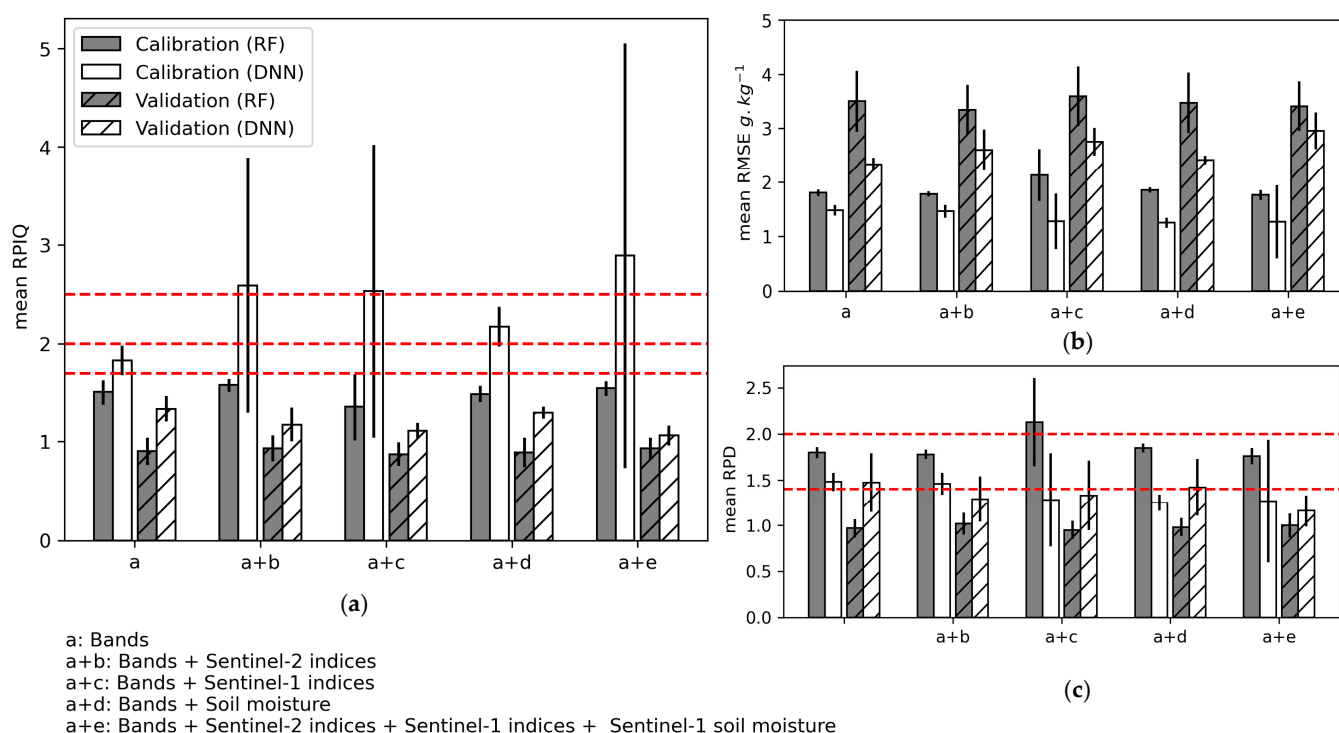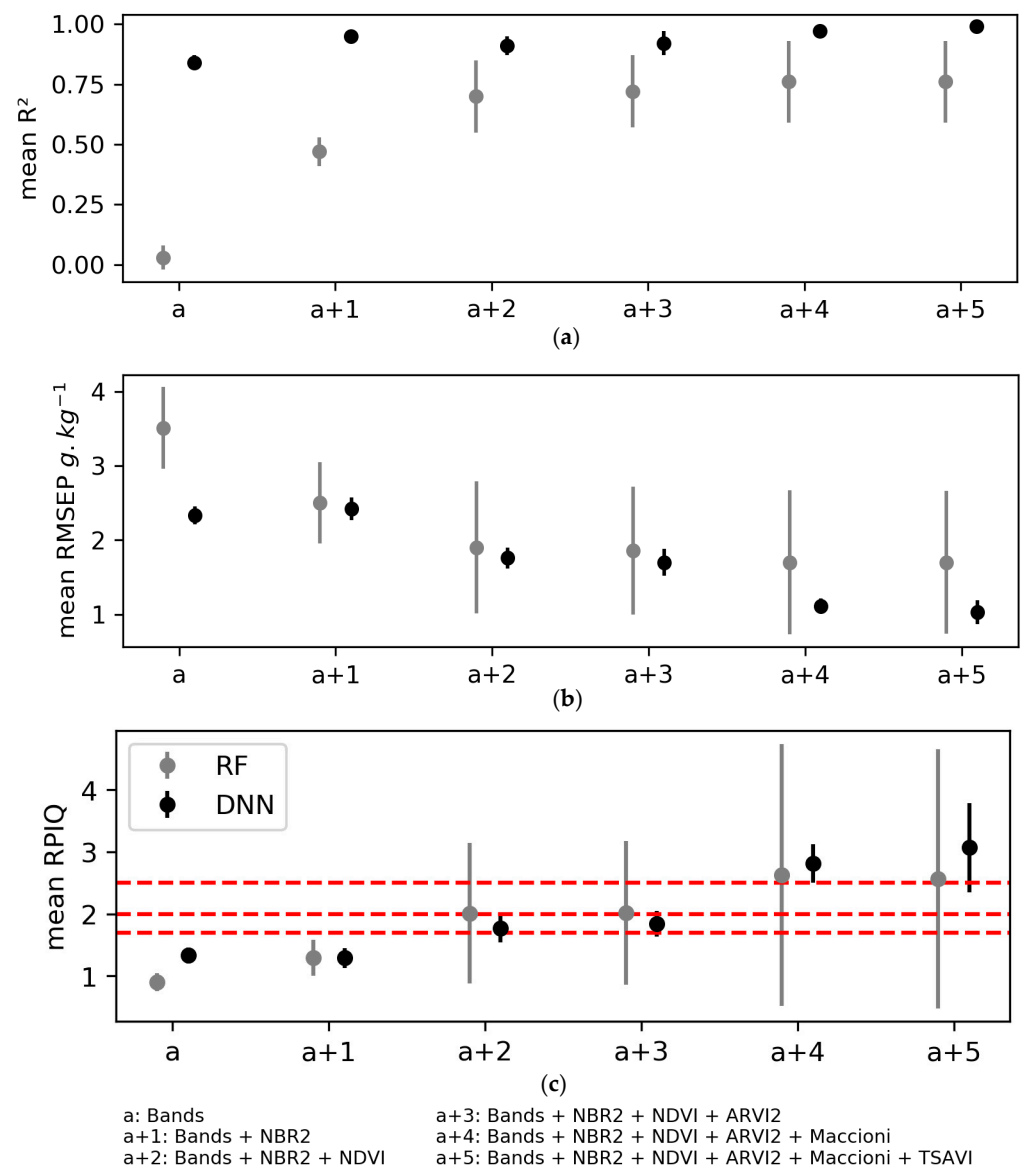a+5: Bands + NBR2 + NDVI + ARVI2 + Maccioni + TSAVI

Figure 10. Mean performance of the three iterations of model validation using the random forest (RF) and deep neural network (DNN) algorithms when adding laboratory spectral indices incrementally in the order of decreasing correlation with soil organic carbon content: (**a**) The coefficient of determination R^2; (**b**) The root mean square error of validation (RMSEP); (**c**) The ratio of performance to the interquartile distance (RPIQ). Error bars indicate 1 standard deviation. Horizontal red lines indicate performance thresholds (see Section 2.6.4). See Table 2 for definitions of the spectral indices.

4. Discussion

4.1. Factors That Influenced Sentinel-2 Soil Surface Reflectance Spectra

The lower reflectance obtained by Sentinel-2 was observed in most previous studies [33,61] and is related to the acquisition conditions: in particular, atmospheric water, soil moisture, and soil roughness. These parameters strongly influence the energy that is reflected and emitted, which reduces reflectance over the entire spectrum [15,17,112] compared to the laboratory spectra acquired after samples were air-dried, sieved to 2 mm, and oven-dried for 24 h. The variability in this information resulted from the diversity of soils and differences in acquisition conditions among dates, since Sentinel-2 reflectance depends on soil complexity, soil surface conditions, and acquisition conditions. To retrieve the relevant information in the images, all Sentinel-2 spectra that corresponded to bare soil for each sample were grouped in a single table, which can provide an alternative to the

mosaicking approaches developed in previous studies [28,38,113]. Vaudour et al. [38] found that temporal mosaicking approaches increased the predicted area but did not predict SOC content better than single-date models. This is because soil conditions, such as soil moisture, soil roughness, and vegetation significantly influence prediction performance by disturbing soil reflectance [31]. Considering Sentinel-2 images acquired on different dates allows one to assess the ability of models to represent different soil conditions and, thus, increase the number and composition of training sample datasets.

4.2. Performance of Calibrated Models Using Only Sentinel-2 Bands: DNN vs. PLS and RF

When using only Sentinel-2 bands, calibrated DNN models outperformed PLS and RF models for all three iterations. These results are consistent with previous studies that found that DNN models are more suitable for predicting SOC due to their ability to capture complex relationships through multiple hidden layers and neurons [61,105,107]. In addition, DNN models can model complex data. For example, Odebiri et al. [105] found that a DNN model improved the prediction of SOC at the national scale, even when using a dataset with high spatial uncertainty (i.e., multiple scales of variation, different sampling sources, and different acquisition dates). Moreover, DNN models in the present study were less sensitive to high-leverage samples (Figure 8) than PLS and RF models were. The low performance of the PLS regression was expected since PLS models are sensitive to highly leveraged samples, which are generally considered as outliers [114]. Although RF models showed RMSEcv of 1.73–1.85 $g \cdot kg^{-1}$ and fair RPIQ values (RPIQ = 1.41–1.53), validation performance was very poor (RMSEP = 3.51 $g \cdot kg^{-1}$ (± 0.45) and RPIQ = 0.90 (± 0.11)). Thus, several studies have found that RF predicted better than other machine-learning techniques, but others have found that the performance of RF classifiers was sensitive to training samples and data dimensions [115]. Compared to the study of Biney et al. [35], our DNN models (R^2 = 0.18–0.65 and RPIQ = 1.21–1.46) outperformed their PLS, SVM, CR, and ensemble models developed at the field scale (R^2 = 0.11–0.27 and RPIQ = 1.22–1.31). Our models yielded RMSEP of 2.33 $g \cdot kg^{-1}$ (± 0.1), which is better than those obtained by Dvorakova et al. (2023) [116], RMSE = 3.5 $g \cdot kg^{-1}$ (± 0.3), for SOC content ranging from 7.2 to 14.2 $g \cdot kg^{-1}$ and Vaudour et al. (2021) [38], and RMSE = 3.02–5.86 $g \cdot kg^{-1}$ for SOC content ranging from 7.04 to 31.9 $g \cdot kg^{-1}$, in cross validation.

4.3. Effects of Additional Information on Model Calibration and Validation

Including additional information, in particular S2-indices, S1-indices, and S1-soil moisture, was intended to increase the models' predictive performance by providing new variables that distinguish the varying soil conditions better on different acquisition dates. This additional information had more influence during calibration than validation and on the DNN models than on the RF models (e.g., when including S2-indices, mean RPIQ improved from 2.02 (± 0.15) to 2.59 (± 1.30) when calibrating the DNN model and from 1.50 (± 0.13) to 1.57 (± 0.07) when calibrating the RF model) (Figure 9). It likely had more influence during calibration than validation because the validation dataset contained spectral information acquired on dates when soil surface conditions of the sampling points in the training dataset were unknown. In fact, some of the sampling points were bare soil on only a few dates (e.g., 1–3), while others were bare soil on 5–18 dates, which gave the machine-learning algorithms, especially DNN, more opportunities to learn. This may also explain the instability in performance of calibrated DNN models "a + b", "a + c", and "a + e" among the iterations (mean RPIQ = 2.59 (± 1.30), 2.53 (± 1.49), and 2.89 (± 2.16), respectively). Thus, the number of dates retained for each sampling point during model calibration strongly influenced model performance. The additional information may have had stronger effects on the DNN models due to their ability to learn and extract more representative features through their hidden layers and neurons [105,107]. Thus, the validation performance of DNN models that included additional information, varied from 2.41 to 2.95 $g \cdot kg^{-1}$ for RMSEP and from 1.29 to 1.42 for RPD; however, the performance of RF models was almost stable (RMSEP = 3.34–3.59 $g \cdot kg^{-1}$ and RPD = 0.95–1.02).

4.4. Utility of Including Sentinel-2 Spectral Indices

The higher variability, in some S2-indices than others (Figure 5), supports the idea that these indices can distinguish soil surface conditions. For example, the NDVI and Maccioni indices, both developed to detect green vegetation [70,82], showed different variation ranges. Since we selected only bare soils, we expected the Maccioni index to vary less than the NDVI, but this was not the case. This supports the assumption that the spectral regions of vegetation indices are sensitive to SOC content [33,117]. Similarly, for NBR and NBR2, which were developed to detect burn severity, NBR varied more than NBR2. Dvorakova et al. [118] and Demattê et al. [119] found that NBR2 was correlated with the presence of crop residues, so they used it with NDVI to select bare soil to predict SOC [18,30,38]. In the present study, performance increased significantly when including S2-indices during calibration but not validation of DNN models. This may have been due to potential variation in correlation between Sentinel-2 bands and their derived S2-indices or the SOC content among dates depending on soil surface conditions. For example, Gholizadeh et al. [33] observed that the correlation between Sentinel-2 spectral information and SOC content or soil texture varied among study areas.

4.5. Utility of Including Sentinel-1-Derived Data

Since radar signals are sensitive to soil surface conditions, especially soil moisture, soil surface roughness, and vegetation [73,120,121], we included indices derived from the VV and VH polarizations of Sentinel-1 radar signals. Although these indices appeared to be sensitive to vegetation dynamics [74,75], they increased the prediction performance of DNN models during calibration but with high variability among the three iterations, which is consistent with results of Nguyen et al. [51] and Wang et al. [27]. The latter found that including radar-derived data with multispectral data in SOC prediction models increased prediction performance. We also included Sentinel-1-derived soil moisture because we found in a previous study [73] that soil moisture had more influence than soil surface roughness in the Naizin watershed on the Sentinel-1 radar signal because of relatively high soil moisture. Consequently, we assumed that including Sentinel-1-derived soil moisture could increase prediction performance by considering the variability in soil moisture among dates and sampling points, especially since our study area is located on both sides of a stream. This approach resulted in the most stable improvement during model calibration and the closest validation performance to that of models calibrated using only S2 bands, which showed the lowest RMSEP (RMSEP = 2.41 ($\pm$0.08) and 2.33 ($\pm$0.12), respectively), supporting the idea that soil moisture strongly influences the performance of SOC prediction models. Urbina-Salazar et al. [50] found that using Sentinel-2 dates with low soil moisture increased performance of SOC prediction models, but that including soil moisture did not, which was the case for the RF model in our study. Thus, the algorithm used influenced the performance of models calibrated with Sentinel-2 data.

By using all of the complementary information simultaneously, the DNN algorithm was able to extract the most appropriate information for predicting SOC content; thus, this approach provides models with more features, which increases their learning capacity. Wang et al. [27] tested different combinations of Landsat TM- and PALSAR-derived data and found that using six TM bands, six TM-derived indices, and four PALSAR polarizations yielded the best model. In addition, Nguyen et al. [51] found that combining Sentinel-1 C-band dual-polarimetric SAR data and Sentinel-2 optical datasets increased prediction performance.

4.6. Effects of Including Laboratory Spectral Indices

Due to the complex nature of soils, their Vis-NIR spectra aggregate multiple soil chromophore spectral signals [122]. Influenced by many other confounding factors, Sentinel-2 soil reflectance predicted SOC less well than spectra acquired under laboratory conditions [28,33,61]. Thus, as suggested by Ben-Dor et al. [10] and confirmed by Vaudour et al. [32], the predictability of a given soil property using remotely sensed data does not depend solely on the property itself or its spectral behavior as a chromophore. When compar-

ing the performance of Sentinel-2A-derived models for two contrasting agroecosystems, Vaudour et al. [32] found that loading values of the Sentinel-2 bands for a given soil property varied among study areas. Consequently, we included laboratory-acquired soil spectral information, assuming that doing so would provide models with more spectral information about soil properties themselves. In addition, Peng et al. [39] improved maps of predicted SOC content by including geospatial estimates of laboratory soil spectra at 1930 nm. Since spectral indices highlight certain spectral features better, we calculated equivalents of the S2-indices using the soil spectra obtained under laboratory conditions. Similarly, Liu et al. [61] found that these bare soil indices were more accurate in predicting SOC densities than those derived from Sentinel-2 imagery; however, their study relied on a single-date Sentinel-2 image acquired in early winter without describing soil surface conditions. Our results showed strong and significant correlations of these indices with the measured SOC content (Table 5). Furthermore, including these indices sequentially in our models improved the prediction of SOC content. With only two indices, we achieved good performance for both RF and DNN models (mean R^2 = 0.70 (± 0.15) and 0.91 (± 0.04) and mean RPIQ = 2.01 (± 1.13), and 1.77 (± 0.23), respectively). However, the results were less stable for RF than for DNN, even when including five indices. This is consistent with the idea that RF classifiers can be used to classify multisource remote sensing data, mainly due to their computational speed [115], but the fact that they optimize models using only the input datasets identified as important made them unstable in our study. These results suggest that considering the same spectral information acquired in the laboratory for all dates instead of the Sentinel-2 spectral information, which varies as a function of surface conditions, minimizes the effects of surface conditions and highlights the spectral behavior of the soil property itself.

5. Conclusions

This study assessed a new approach for using a time series of Sentinel-2 data combined with Sentinel-1-derived data and Vis-NIR laboratory spectra to predict the SOC content of agricultural soils and tested predictive models of three different algorithms. To retrieve the relevant information contained in the images, all Sentinel-2 spectra that corresponded to bare soil for each soil sample were grouped into a table, which can provide an alternative to mosaicking approaches. Our results showed the following:

The DNN models outperformed the PLS and RF models and the inclusion of additional information (i.e., S2-indices, S1-indices, and S1-soil moisture) influenced the prediction performance of the DNN models more than that of the RF models.

Although the inclusion of additional information improved prediction performance during model calibration, it did not influence model validation. Furthermore, S1-soil moisture gave the most stable improvement in calibration and the closest validation performance to that of models calibrated using only S2 bands, which had the lowest RMSEP.

As the Lab-indices showed strong and significant correlations with measured SOC content, their incremental addition to the models improved the prediction of SOC content, and the addition of only two indices yielded good performances.

Future research could evaluate the approach developed for study areas that have more available Sentinel-2 data and different soil and climate conditions to assess its potential to be generic. Accordingly, the principal objective of this study was to improve the accuracy of SOC content prediction using Sentinel-2 data, with the ultimate goal of producing highly detailed SOC maps. The availability of these maps will be of great help in the crucial issue of monitoring agricultural soils in relation to agricultural practices.

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Data Availability Statement: The data presented in this study are available on request from the corresponding author.

Conflicts of Interest: The authors declare no conflict of interest.

Appendix A

Table A1. Equations for Sentinel-2 spectral indices.

Abbreviation	Index	Equation	Reference
		Vegetation indices	
AFRI16	Aerosol free vegetation index 2.1	$\frac{B8A - 0.66 \times B11}{B8A + 0.66 \times B11}$	[79]
AFRI21	Aerosol free vegetation index 2.1	$\frac{B8A - 0.5 \times B12}{B8A + 0.5 \times B12}$	[79]
ARI	Anthocyanin reflectance index	$\frac{1}{B3} - \frac{1}{B5}$	[123]
ARVI2	Atmospherically Resistant vegetation index2	$-0.18 + 1.17 \times \left(\frac{B8 - B4}{B8 + B4} \right)$	[80]
BRI	Browning reflectance index	$\frac{\frac{1}{B3} - \frac{1}{B5}}{B6}$	[124]
BWDRVI	Blue-wide dynamic range vegetation index	$\frac{0.1 \times B7 - B2}{0.1 \times B7 + B2}$	[125]
CCCI	Canopy chlorophyll content index	$\frac{(B8 - B5)/(B8 + B5)}{(B8 - B4)/(B8 + B4)}$	[126]
EVI	Enhanced vegetation index	$\frac{2.5 \times (B8 - B4)}{(B8 + 6 \times B4 - 7.5 \times B2) + 1}$	[127]
EVI2	Enhanced vegetation index2	$\frac{2.4 \times (B8 - B4)}{(B8 + B4 + 1)}$	[128]
GARI	Green atmospherically resistant vegetation index	$\frac{B8 - (B3 - (B2 - B4))}{B8 + (B3 + (B2 - B4))}$	[129]
GLI	Green leaf index	$\frac{2 \times B3 - B5 - B2}{2 \times B3 + B5 + B2}$	[130]
GNDVI	Green normalized difference vegetation index	$\frac{B8 - B3}{B8 + B3}$	[129]
GVMI	Global vegetation moisture index	$\frac{(B8 + 0.1) - (B12 + 0.02)}{(B8 + 0.1) + (B12 + 0.02)}$	[81]
Maccioni	Maccioni vegetation index	$\frac{B7 - B5}{B7 - B4}$	[82]
NBR	Normalized burn ratio	$\frac{B8 - B12}{B8 + B12}$	[83]
NBR2	Normalized burned Ratio 2	$\frac{B11 - B12}{B11 + B12}$	[84,85]
NDVI	Normalized difference vegetation index	$\frac{B8 - B4}{B8 + B4}$	[70]
NSSI	NPV-soil separation index	$\frac{B8A - B7}{\frac{B8A}{B7}}$	[131]
OSAVI	Optimized soil-adjusted vegetation index	$\frac{B8 - B4}{B8 + B4 + 0.16}$	[132]
PANDVI	Pan normalized difference vegetation index	$\frac{B8 - (B3 + B4 + B2)}{B8 + (B3 + B4 + B2)}$	[133]

Table A1. *Cont.*

Abbreviation	Index	Equation	Reference
SIWSI	Shortwave infrared water stress index	$\frac{B8A - B11}{B8A + B11}$	[86]
TSAVI	Soil-adjusted vegetation index	$\frac{1.22 \times (B8 - 1.22 * B4 - 0.03)}{1.22 \times B8 + B4 - 1.22 \times 0.03 + 0.08 \times (1 + 1.22^2)}$	[87]
Soil indices			
BI	Brightness index	$\sqrt{\frac{B2^2 + B3^2 + B4^2}{3}}$	[89,134]
BSI	Bare soil index	$\frac{(B12 - B4) - (B8 - B2)}{(B12 - B4) + (B8 - B2)}$	[90]
FI	Form index	$\frac{2 \times B4 - B3 - B2}{B3 - B2}$	[135]
Hue	Hue index	$arctan\left(\left(\frac{2 \times B5 - B3 - B2}{30.5}\right) \times (B3 - B5)\right)$	[135]
RedI	Redness index	$\frac{B4^2}{B3^3}$	[89]
SI	Saturation index	$\frac{B4 - B2}{B4}$	[135]
S2WI	Soil moisture index	$\frac{B8 - B11 - B12}{B8 + B11 + B12}$	[32]
STI	Soil tillage index	$\frac{B11}{B12}$	[136]
Geology indices			
Fe2	Ferrous iron index	$\frac{B12}{B8} - \frac{B3}{B4}$	[137]
Fe3	Ferric iron index	$\frac{B3}{B4}$	[137]
FO	Ferric oxides index	$\frac{B11}{B8}$	[137]
FS	Ferrous silicates index	$\frac{B12}{B11}$	[137]
Gossan	Gossan index	$\frac{B11}{B4}$	[137]
Water indices			
AWEI	Automated water extraction index not dominant shadow	$4 \times (B3 - B11) - (0.25 \times B8 + 2.75 \times B12)$	[121]
AWEI2	Automated water extraction index dominant shadow	$B2 + 2.5 \times B3 - 1.5 \times (B8 + B1) - 0.25 \times B12$	[138]
MNDWI	Modified normalized difference water index	$\frac{B3 - B11}{B3 + B11}$	[139]
NDMI	Normalized difference moisture index	$\frac{B8 - B11}{B8 + B11}$	[91]
NDWI	Normalized difference water index	$\frac{B3 - B8}{B3 + B8}$	[140]

Appendix B

Table A2. Adjusted parameters for models when using only Sentinel-2 bands and when including Sentinel-2 indices, Sentinel-1 indices, and/or Sentinel-1 soil moisture.

Input		PLS			RF		DNN
	It.	Factors	Scale	Max_Features	Max_Depth		Num_Layers
a	(1)	6	True	0.60	70		12
	(2)	5	False	auto	10		8
	(3)	6	True	0.60	70		7
a + b	(1)	-	-	0.75	20		10
	(2)	-	-	0.60	30		5
	(3)	-	-	0.85	70		12
a + c	(1)	-	-	0.95	50		12
	(2)	-	-	0.85	10		11
	(3)	-	-	0.85	10		12
a + d	(1)	-	-	0.6	None		5
	(2)	-	-	0.85	10		9
	(3)	-	-	0.60	None		9
a + e	(1)	-	-	0.60	70		13
	(2)	-	-	0.60	30		13
	(3)	-	-	0.60	None		13

Table A3. Detailed performance of models calibrated using only Sentinel-2 bands with the partial least squares (PLS) regression, random forest (RF), or deep neural network (DNN) algorithms (Alg.) for the three iterations (It.) ((1), (2), and (3)).

Alg.	It.	R^2	Calibration RMSECV	RPD	RPIQ	r^2	Validation RMSEP	RPD	RPIQ
PLS	(1)	0.15	3.27	1.08	0.79	0.13	3.58	1.07	0.93
	(2)	0.15	3.21	1.08	0.83	0.06	3.88	1.03	0.77
	(3)	0.17	3.67	1.1	0.77	−0.10	2.61	0.95	1.15
RF	(1)	0.73	1.82	1.94	1.41	0.09	3.65	1.05	0.91
	(2)	0.75	1.73	2.00	1.54	0.02	3.96	1.01	0.76
	(3)	0.79	1.85	2.17	1.53	−0.34	2.88	0.86	1.04
DNN	(1)	0.81	1.55	2.29	1.67	0.65	2.28	1.69	1.46
	(2)	0.85	1.36	2.55	1.96	0.62	2.47	1.62	1.21
	(3)	0.86	1.53	2.63	1.86	0.18	2.25	1.11	1.33

Table A4. Detailed performance for the three iterations (It.) ((1), (2), and (3)) of the calibrated random forest (RF) and deep neural network (DNN) models and their validation when including Sentinel-2 indices, Sentinel-1 indices, and/or Sentinel-1 soil moisture.

| | | RF Calibration | | | | | Validation | | | DNN Calibration | | | | | Validation | | |
Input	It.	R^2	RMSECV	RPD	RPIQ	r^2	RMSEP	RPD	RPIQ	R^2	RMSE	RPD	RPIQ	r^2	RMSEP	RPD	RPIQ
a	(1)	0.73	1.82	1.94	1.41	0.09	3.65	1.05	0.91	0.81	1.55	2.29	1.67	0.65	2.28	1.69	1.46
	(2)	0.75	1.73	2.00	1.54	0.02	3.96	1.01	0.76	0.85	1.36	2.55	1.96	0.62	2.47	1.62	1.21
	(3)	0.79	1.85	2.17	1.53	−0.34	2.88	0.86	1.04	0.86	1.53	2.63	1.86	0.18	2.25	1.11	1.33
a + b	(1)	0.76	1.74	2.03	1.48	0.18	3.47	1.11	0.96	0.86	1.33	2.66	1.94	0.56	2.55	1.51	1.31
	(2)	0.72	1.83	1.90	1.46	0.13	3.73	1.07	0.8	0.81	1.53	2.27	1.74	0.43	3.01	1.33	0.99
	(3)	0.8	1.78	2.26	1.60	−0.30	2.83	0.88	1.06	0.97	0.70	5.87	4.08	0.02	2.46	1.02	1.22
a + c	(1)	0.43	2.67	1.33	0.97	0.04	3.76	1.02	0.89	0.82	1.51	2.35	1.71	0.44	2.87	1.34	1.16
	(2)	0.74	1.78	1.96	1.50	−0.02	4.04	0.99	0.74	0.78	1.64	2.11	1.62	0.46	2.93	1.37	1.02
	(3)	0.77	1.93	2.08	1.47	−0.44	2.98	0.83	1.00	0.97	0.67	6.02	4.25	−0.11	2.61	0.95	1.14
a + d	(1)	0.72	1.87	1.90	1.38	0.09	3.66	1.05	0.91	0.86	1.33	2.67	1.94	0.59	2.47	1.56	1.35
	(2)	0.73	1.80	1.93	1.49	0.03	3.92	1.02	0.76	0.89	1.15	3.01	2.32	0.63	2.44	1.64	1.23
	(3)	0.78	1.89	2.13	1.51	−0.30	2.84	0.87	1.05	0.9	1.26	3.2	2.26	0.13	2.32	1.07	1.29
a + e	(1)	0.75	1.78	1.99	1.45	0.16	3.51	1.09	0.95	0.81	1.56	2.28	1.66	0.31	3.2	1.21	1.04
	(2)	0.77	1.66	2.10	1.61	0.09	3.81	1.05	0.78	0.98	0.50	7.01	5.38	0.4	3.08	1.30	0.97
	(3)	0.79	1.84	2.18	1.54	−0.37	2.91	0.85	1.03	0.81	1.75	2.3	1.63	−0.06	2.56	0.97	1.17

a: Bands, a + b: Bands + Sentinel-2 indices, a + c: Bands + Sentinel-1 indices, a + d: Bands + Soil moisture, a + e: Bands + Sentinel-2 indices + Sentinel-1 indices + Sentinel-1 soil moisture.

Table A5. Adjusted parameters for models when adding laboratory spectral indices incrementally in the order of decreasing correlation with soil organic carbon content.

Input	It.	RF Max_Features	Max_Depth	DNN Num_Layers
a	(1)	0.60	70	12
	(2)	auto	10	8
	(3)	0.60	70	7
a + 1	(1)	auto	70	11
	(2)	Auto	10	10
	(3)	auto	20	10

Table A5. *Cont.*

Input	It.	RF Max_Features	RF Max_Depth	DNN Num_Layers
a + 2	(1)	0.85	10	7
	(2)	auto	30	6
	(3)	auto	30	12
a + 3	(1)	0.58	50	12
	(2)	auto	30	11
	(3)	auto	70	3
a + 4	(1)	auto	10	11
	(2)	0.95	None	12
	(3)	0.95	None	12
a + 5	(1)	auto	20	13
	(2)	auto	30	9
	(3)	0.95	30	5

Table A6. Detailed performance for the three iterations (It.) ((1), (2), and (3)) of the calibrated random forest (RF) and deep neural network (DNN) models and their validation when adding laboratory spectral indices incrementally in the order of decreasing correlation with soil organic carbon content.

Input	It.	RF Calibration R^2	RMS ECV	RPD	RPIQ	RF Validation r^2	RMS EP	RPD	RPIQ	DNN Calibration R^2	RMSE	RPD	RPIQ	DNN Validation r^2	RMS EP	RPD	RPIQ
a	(1)	0.73	1.82	1.94	1.41	0.09	3.65	1.05	0.91	0.73	1.55	2.29	1.67	0.65	2.28	1.69	1.46
	(2)	0.75	1.73	2.00	1.54	0.02	3.96	1.01	0.76	0.75	1.36	2.55	1.96	0.62	2.47	1.62	1.21
	(3)	0.79	1.85	2.17	1.53	−0.34	2.88	0.86	1.04	0.79	1.53	2.63	1.86	0.18	2.25	1.11	1.33
a + 1	(1)	0.81	1.53	2.32	1.69	0.43	2.89	1.33	1.15	0.96	0.69	5.18	3.76	0.65	2.27	1.7	1.47
	(2)	0.82	1.45	2.39	1.84	0.53	2.74	1.46	1.09	0.96	0.67	5.17	3.97	0.59	2.56	1.56	1.17
	(3)	0.86	1.50	2.68	1.90	0.44	1.87	1.33	1.60	0.94	0.95	4.23	2.99	0.04	2.43	1.02	1.23
a + 2	(1)	0.83	1.47	2.42	1.76	0.57	2.52	1.52	1.32	0.96	0.69	5.14	3.75	0.82	1.64	2.35	2.03
	(2)	0.79	1.58	2.20	1.69	0.67	2.30	1.74	1.30	0.88	1.20	2.91	2.23	0.77	1.92	2.09	1.56
	(3)	0.86	1.46	2.74	1.94	0.87	0.88	2.82	3.40	0.90	1.25	3.22	2.27	0.52	1.72	1.45	1.74
a + 3	(1)	0.79	1.61	2.21	1.61	0.58	2.50	1.54	1.33	0.87	1.27	2.79	2.02	0.8	1.73	2.22	1.92
	(2)	0.82	1.45	2.40	1.84	0.70	2.20	1.81	1.36	0.97	0.62	5.60	4.30	0.78	1.86	2.16	1.61
	(3)	0.87	1.44	2.79	1.97	0.87	0.89	2.79	3.36	0.92	1.16	3.46	2.44	0.63	1.50	1.66	1.99
a + 4	(1)	0.84	1.41	2.52	1.83	0.61	2.39	1.61	1.39	0.95	0.78	4.54	3.30	0.92	1.10	3.51	3.04
	(2)	0.83	1.41	2.46	1.89	0.72	2.11	1.89	1.42	0.99	0.40	8.75	6.72	0.93	1.02	3.92	2.92
	(3)	0.88	1.36	2.96	2.06	0.94	0.59	4.21	5.07	0.96	0.81	4.98	3.52	0.76	1.21	2.05	2.46
a + 5	(1)	0.84	1.40	2.53	1.84	0.60	2.42	1.59	1.38	0.99	0.21	16.74	12.17	0.95	0.85	4.51	3.90
	(2)	0.83	1.43	2.42	1.86	0.73	2.08	1.92	1.44	0.99	0.34	10.21	7.84	0.92	1.10	3.65	2.72
	(3)	0.89	1.32	3.04	2.15	0.94	0.61	4.07	4.90	0.99	0.46	8.65	6.11	0.78	1.15	2.16	2.59

a: Bands, a + 1: Bands + NBR2, a + 2: Bands + NBR2 + NDVI, a + 3: Bands + NBR2 + NDVI + ARVI2; a + 4: Bands + NBR2 + NDVI + ARVI2 + Maccioni, a + 5: Bands + NBR2 + NDVI + ARVI2 + Maccioni + TSAVI.

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