Soil organic carbon prediction using visible–near infrared reflectance spectroscopy employing artificial neural network modelling

Justin George, K.*, Suresh Kumar and R. Arya Raj

Agriculture and Soils Department, Indian Institute of Remote Sensing (ISRO), 4 Kalidas Road, Dehradun 248 001, India

Visible–near infrared (VNIR) spectroscopy is a relatively fast and cost-effective analytical technique for estimating soil organic carbon (SOC). The present study was undertaken for predicting SOC using VNIR reflectance spectroscopy employing artificial neural network (ANN). Surface soil samples (0–15 cm) were collected from 75 georeferenced locations through grid sampling approach in a hilly watershed of Himachal Pradesh, India, and analysed for SOC. The reflectance spectra of soil samples was measured using a spectroradiometer in the wavelength range of 350–2500 nm. Various spectral indices were generated using the sensitive bands in the visible region. The SOC-sensitive spectral indices and reflectance transformations were utilized for predictive modelling of SOC using the ANN model. This model could predict SOC values with $R^2$ of 0.92 and MSE value of 0.24, indicating that this technique can be used to predict SOC in a spatial domain when coupled with high-resolution hyperspectral satellite/airborne data.

Keywords: Artificial neural network model, reflectance spectroscopy, soil organic carbon, visible and near infrared region.

Soil organic carbon (SOC) plays a fundamental role in determining the physical, chemical and biological properties of the soil. It is beneficial for maintaining soil productivity, water-holding capacity as well as carbon sequestration for alleviating the ill-effects of greenhouse gases and thus climate change. Conventional methods for SOC determination in soil laboratories are costly, time-consuming and may be environmentally hazardous. Thus there is an urgent need for the development of fast, accurate and non-destructive methods (thus reducing the number of soil chemical analyses) for SOC estimation, which will help in generating high-resolution soil property maps of large areas at modest costs.

*For correspondence. (e-mail: justin@iirs.gov.in)
Visible–near infrared (VNIR) spectroscopy has been identified as a relatively fast and cost-effective technique for various agricultural paradigms. Spectroscopy has proved its potential to accurately determine SOC in the laboratory as well as in the field where nondestructive imaging can be performed. Viscarra Rossel et al. showed that NIR spectroscopy can estimate several primary and secondary soil properties like SOC, total N and Ca, K and Mn. The electromagnetic range of 400–2500 nm in spectroscopy enables accurate prediction of SOC due to its influence on the shape and magnitude of the reflectance spectrum. Zhuo et al. mapped SOC utilizing a spectrometer and also used spectra from the laboratory to map the physical and chemical properties of the soil with special emphasis on its characteristic absorption bands. Also, the potentiality of spectroscopy in mapping and quantifying a wide range of soil properties was reviewed by Ben-Dor et al., as an effective tool for advanced soil mapping studies. NIR spectroscopy using field- and space-borne sensors enables direct mapping of soil properties and assessment of soil quality. This capability of field or laboratory spectra was shown to be ideal for soil-related studies. An ASD spectrometer was also successfully used for estimating soil carbon, nitrogen, carbonate and organic matter in various horizons of the soil profile from different sites in Washington and Oregon, USA, at 400–1000 nm using the regression tree model.

Artificial neural network (ANN), an effective data mining technique, was found to give better results in predicting SOC content, clay content and soil pH than other regression and statistical techniques. This may be due to its strong connectivity of networks that could possibly draw out an effective relationship between soil properties and spectral features. Also, the soil map derived using ANN was found to be more accurate than all other conventional methods of soil mapping. ANN uses various supervised networks like feed-forward neural network (FFN) with backpropagation network architecture, which acts as a channel where the output defines the pattern and function of the network channel leading to inputs, which can be further used reversely with known inputs to derive unknown outputs. Multilayer feedback propagation algorithms facilitate ANN training in a more effective way, and these were utilized for estimating soil nutrients like phosphorus using DEM-derived terrain attributes, which proved the suitability of ANN in quantitative prediction of soil nutrients. Therefore, the present study was undertaken to verify the possibility of employing ANN modelling for predicting SOC using VNIR reflectance spectroscopy.

The study was conducted in a watershed located in the mid-Himalayan region of Mandi district, Himachal Pradesh (lat. 32°4′35.04″–32°1′3.8964″N and long. 76°39′49.60″–76°44′15.84″E), India, covering a total geographical area of 1000 ha (10 km²). Nearly 80% of the watershed is comprised of agricultural fields where rice and wheat are the major crops grown. Figure 1 shows the complete methodology adopted in the study. To properly represent soil spatial variability in the watershed and ensure unbiased and precise sampling, grid sampling approach was used for soil sample collection, with a grid size of 250 m × 250 m on ground. Georeferenced surface soil samples (0–15 cm) were collected from 75 locations in the watershed during November 2015, when the fields were fallow. The soil samples were air-dried, preprocessed and divided into two parts, one part for analysis of SOC as well as basic soil physio-chemical characteristics, and other for the generation of reflectance spectra in the laboratory. Preprocessed and 0.2 mm sieved soil samples were used for the estimation of SOC (TOC analyzer). Based on analytical results, soils in the watershed were found to be predominantly acidic in nature with pH values ranging from 4.34 to 5.61 (mean value of 4.85). The electrical conductivity (EC) values were very low, indicating that the soils are devoid of soluble salts/salinity. Soils in the area were found to be loamy in texture, predominantly belonging to silt loam and sandy loam textural classes. The samples were found to have medium to high SOC content, with majority of the values greater than 0.5%. The SOC values ranged from 0.26 to 2.71 g kg⁻¹ soil, with a mean value of 1.36 g kg⁻¹ soil. The soils belonged to moderate to well drainage class.

The surface reflectance spectra of the preprocessed soil samples in the wavelength range 350–2500 nm were
measured in the laboratory using a spectroradiometer (ASD FieldSpec Pro Spectroradiometer), under controlled dark-room conditions. Precautions were taken to avoid stray light as well as dark current generated within the instrument. Also, the instrument was calibrated using white reference panel at the start as well as after every five successive reflectance measurements. The spectra were collected as an average of 25 readings for each sample, with a spectral resolution of 1 nm, after real-time viewing. For each sample data, five spectra were collected and averaged out for generating spectral libraries. The spectra collected at 1 nm interval were also resampled to 5 nm interval using the spectral resampling tool in ENVI 5.0 for further analysis.

Sensitive spectral bands specific to SOC were studied through a literature survey\textsuperscript{12,21–23}. Various bands identified for their sensitivity to SOC were 400, 441, 520, 907, 960, 1100, 1720, 1744, 1870, 2052, 2180 and 2309 nm. Correlation between selected spectral bands and SOC data was done, and the sensitive bands were identified. In the visible range (400–700 nm), spectra were divided into three regions, i.e. blue (400–500 nm), green (500–600 nm) and red (600–700 nm), for analysis and identification of the most sensitive bands within each of the three regions. For rest of the spectra, only bands identified from the literature were used for analysis.

The spectral bands selected through correlation analysis were used to generate spectral indices. Five nanospectral indices were developed, namely brightness index (BI), colouration index (CI), saturation index (SI), redness index (RI) and hue index (HI) (eqs 1–5). These are colouration indices, which are sensitive to soil colour, these indices were chosen for the present study. The indices make use of blue, green and red wavelength regions in the visible range; hence single nanobands in these regions having highest correlation coefficient ($r$) were selected for developing the indices. Reflectance values at 451 nm, 520 nm and 690 nm representing blue, green and red regions respectively were selected (Table 1). The indices derived were then used for correlation analysis with SOC. The bands in the shortwave IR region, especially 2180 and 2309 nm, were also found to have higher correlation with SOC values (Table 1). Owing to the significance of the NIR region in predicting SOC, bands in this region along with the first derivative, second derivative and logarithmic values, reciprocal of logarithmic values and reciprocals of derivatives were also subjected to correlation analysis.

\begin{align*}
\text{BI} &= \sqrt{\left(\text{Blue}^2 + \text{Green}^2 + \text{Red}^2\right)/3}, \quad (1) \\
\text{CI} &= \frac{(\text{Red} - \text{Green})}{(\text{Red} + \text{Green})}, \quad (2) \\
\text{HI} &= \frac{(2 \times \text{Red} - \text{Green} - \text{Blue})}{(\text{Green} - \text{Blue})}, \quad (3)
\end{align*}

where 451, 520 and 690 nm wavelengths represent the blue, green and red bands respectively.

The ANN modelling for SOC prediction was executed using Matlab software Ver 2015. The nano-spectral indices that showed good correlation with SOC were used for analysis (Table 2). In addition, the reciprocal of first derivative of reflectance value at wavelength 2309 nm and reflectance value of the 2180 nm band showed high correlation coefficient and were also taken as input to the ANN. The data preparation and subsequent database generation were done in Excel and the neural network was executed using Neural Network Tool in Matlab. The entire soil dataset was separated into two datasets – calibration (50 nos) and validation (25 nos) datasets using random numbers. During the model training and development phase, the calibration set was further internally separated into 3 sub-datasets, i.e. training (68%), validation (16%) and testing (16%) datasets.

A multilayer FFN consisting of input, hidden and output layers known for its better performance in solving intricate input-output relationship was used for the prediction of SOC. To circumvent overtraining issue coupled with FFN, we used back-propagation algorithm for network training, which is recognized for its easy execution. ANNs are known for their capability to model and represent functions of nonlinear nature. A tan–sigmoid function known to proximate nonlinear interactions between inputs and outputs was chosen as the transfer function for the hidden and output layers\textsuperscript{25}. Overall network was trained using the Levenberg–Marquardt algorithm\textsuperscript{26} and its performance was evaluated using $R$ values from regression plots. The developed ANN model was

\begin{align*}
\text{RI} &= \text{Red}^2 + (\text{Blue} \times \text{Green}^3), \quad (4) \\
\text{SI} &= \frac{(\text{Red} - \text{Blue})}{(\text{Red} + \text{Blue})}, \quad (5)
\end{align*}
further employed for prediction of SOC values corresponding to the input variables of validation dataset. The SOC prediction accuracy of the model was evaluated using the coefficient of determination \( (R^2) \) and MSE (mean square error) values.

Based on the results of Pearson correlation test, seven variables (CI, BI, HI, SI, RI, \( R_{2180} \) and reciprocal of the first derivative of \( R_{2309} \)) were selected for predictive modelling of SOC using ANN. Thus, the designed ANN network had seven input layers corresponding to the

Figure 2. Regression plot of the accepted artificial neural network model.

Figure 3. Observed versus predicted plot of soil organic carbon values.
various predictive variables. Based on the trial and error method suggested by Chiang et al., the number of neurons in the hidden layer of the network for prediction of SOC was optimized to be 12. The training of the network was assessed using the regression plots of training, validation, testing (three sub-datasets) and total calibration dataset, exhibiting $R^2$-values (Figure 2). Network training using the data was done until $R^2$-values of all the three sub datasets were greater than 0.9 or close to 1. The well-calibrated model was employed for the prediction of SOC values using the validation dataset. Using the well-trained ANN model, we were able to precisely predict SOC values with an $R^2$ of 0.92 and MSE of 0.24 (Figure 3).

This study demonstrates that VNIR spectroscopy can be an effective tool for quantitative prediction of various soil nutrients, especially SOC. This SOC prediction model developed using soil samples from a mid-Himalayan watershed could be used for effective characterization and soil nutrient prediction in other regions as well. This nondestructive prediction model could help in the real-time evaluation of SOC, when coupled with high-resolution hyperspectral satellite/airborne data, enabling farmers to adopt precision farming for sustainable agricultural production.

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