Dependency Measures for Assessing the Covariation of Spectrally Active and Inactive Soil Properties in Diffuse Reflectance Spectroscopy

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Diffuse reflectance spectroscopy (DRS) is a rapid and noninvasive assessment technique for several spectrally active soil properties (chromophores) such as sand, clay, organic C, and Fe contents. The approach is also used for estimating many spectrally inactive constituents (non-chromophores) based on the assumption of covariation between non-chromophores and chromophores. The linkage between covariation and the ability of DRS to estimate a non-chromophore has not been reported in the literature. In this study, we evaluated the covariation assumption using three dependency measures (Pearson correlation coefficient, *r*; biweight midcorrelation, bicor; and mutual information based adjacency, AMI), five chromophores (organic C, Fe, clay, and sand contents, and geometric mean diameter), and seven non-chromophores (pH, electrical conductivity, P, K, B, Zn, and Al contents) measured in 247 Alfisol and 249 Vertisol samples. An average dependency index (ADI) was developed for each of the three measures (ADI_r, ADI_{bicor}, and ADI_{AMI}). The first derivative of the reflectance in conjunction with partial least squares regression was used for data modeling. Model accuracy was evaluated using residual prediction deviation (RPD). The relationships between RPD values of non-chromophores and the ADI values were examined for different chromophore groups (physical, chemical, and combined). The performance of ADI_{AMI} was found to be superior to ADI_r and ADI_{bicor}. The ADI_{AMI} computed using chemical chromophores gave strong linear relationships ($R^2 = 0.93$) between ADI_{AMI} and the RPD of chemical non-chromophores, suggesting that the AMI may be used as a robust dependency measure to assess the covariation of non-chromophores with chromophores in DRS.

Abbreviations: AMI, adjacency values of mutual information; bicor, biweight midcorrelation, DRS, diffuse reflectance spectroscopy; EC, electrical conductivity; FD, first derivative; GMD, geometric mean diameter; MI, mutual information; OC, organic carbon; PLSR, partial least squares regression; RPD, residual prediction deviation; VNIR, visible to near infrared.

Rapid and reliable assessment of soil characteristics has become a mainstream component for monitoring and management of agricultural and natural resources. Soil properties vary widely both in time and space (Cohen et al., 2005; Minasny and Hartemink, 2011). Even with decades of research and development, the in situ and frequent assessment of different soil properties remains a formidable task. Remote sensing tools appear to be a feasible technology to provide a comprehensive solution to this problem (Vasques et al., 2010). Specifically, the diffuse reflectance spectroscopy (DRS) technique in the visible to near-infrared (VNIR) regions (350–2500 nm) has emerged as a rapid and noninvasive technique for the estimation of soil properties (Ben-Dor et al., 2009). Two

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of the most attractive advantages of the DRS approach are (i) that it has the potential to replace the cumbersome and expensive chemical analyses procedures used in soils and (ii) that it is amenable to both proximal and remote sensing mode of operations (Viscarra Rossel et al., 2006).

The uniqueness of the DRS technique is its capability to estimate a range of soil properties from a single reflectance spectrum of the soil by means of regression models. The DRS approach has been used for estimating soil texture (Volkan Bilgili et al., 2010), organic C (OC) contents (Galvao and Vitorello, 1998; Fox and Metla, 2005; Singh et al., 2013), nutrient contents including N (Vågen et al., 2006), P, and K (Mouazen et al., 2007), electrical conductivity (EC) (Shrestha, 2006), cation exchange capacity (CEC) (Fox and Metla, 2005), Fe content (Galvao and Vitorello, 1998), color (Mathieu et al., 1998), soil moisture contents (Whiting et al., 2004), carbonates (Gomez et al., 2008), mineralogical composition (Clark, 1999), hydraulic properties (Santra et al., 2009), and parameters for the aggregate size distribution function (Sarathjith et al., 2014) among others. The DRS models are generally evaluated using the residual prediction deviation (RPD) criterion (Chang et al., 2001), which is defined as

$$\mathrm{RPD}=\left(\frac{1/(n-1)\sum_{i=1}^{n}\left(Y_i-\overline{Y}\right)^2}{1/n\sum_{i=1}^{n}\left(Y_i-\hat{Y}_i\right)^2}\right)^{1/2}_{\text{Validation}} \qquad [1]$$

where Y_i and $\hat{Y}_i$ are the observed and predicted response variables, respectively, $\overline{Y}$ is the mean of the Y_i values, and n is the number of soils in the validation data set. Chang et al. (2001) classified prediction accuracies into accurate (RPD > 2), moderate (1.4 < RPD < 2), and poor (RPD < 1.4), although such a rule is still being debated (Bellon-Maurel et al., 2010).

Spectral reflectance (R) across the VNIR region of a soil is a collective response caused by the molecular vibrations of specific soil constituents and scattering phenomena because of the aggregated nature of soil particles (Ben-Dor, 2011). Specifically, the magnitude of R at a specific wavelength (l) is chemically influenced by the electronic transitions, overtones, and combinations of Fe-bearing minerals, clay minerals, and C–H functional groups of organic matter contents (Clark, 1999) and physically influenced by the extent of scattering and self-shadowing effects of the surface roughness (Baumgardner et al., 1985). Thus, chemical constituents such as clay minerals, Fe oxides, OC content, and moisture content are referred to as spectrally active components or simply chemical chromophores. The physical chromophores mainly consist of those factors affecting the diffusion of light in soil, such as texture, aggregate size distribution, roughness, porosity, etc. In addition to these spectrally active components, the DRS approach is also used for estimating several spectrally inactive soil attributes such as pH (Abdi et al., 2012; Viscarra Rossel and Webster, 2012), micronutrients such as Zn (Abdi et al., 2012), and major nutrients such as P, K, and S (Malley et al., 1999) among others. Although the term *chromophore* strictly applies to the functional groups influenced by the optical region of the reflectance spectra, we adopt the definition of Ben-Dor (2011) and refer to all spectrally active components of soil as chromophores and spectrally inactive components as non-chromophores. The success of estimating non-chromophores by the DRS approach is advocated as an outcome of the covariation of a non-chromophore with relevant chromophores (Stenberg et al., 2010). Hence, it was hypothesized that if the assumption of covariation is valid, then the strength of covariation may be linked with the predictability of non-chromophores.

Two popular ways of assessing the covariation assumption are by (i) comparing the prediction of a non-chromophore by the DRS approach and the pedotransfer function (PTF) approach (Bouma, 1989; Santra and Das, 2008), where non-chromophores are expressed as linear combinations of chromophores through multiple linear regression (MLR) models (Chang et al., 2001), or (ii) computing the Pearson correlation coefficient (r) between non-chromophores and chromophores (Nduwamungu et al., 2009; Volkan Bilgili et al., 2010; Abdi et al., 2012; Kinoshita et al., 2012) measured under laboratory conditions. Chang et al. (2001) observed that both DRS and PTFs yielded similar predictability for CEC and Cu, whereas the predictabilities by these two approaches were different for non-chromophores such as pH, K, and Mn. The inefficacy of MLR to accurately represent the relationship between chromophores and non-chromophores may be one of the reasons for the dissimilar predictability. In the second approach, the prediction of a non-chromophore has been linked with the magnitude of r values with chromophores. Abdi et al. (2012) showed that the accurate prediction of pH (RPD = 3.23) was due to its correlation with both total C (r = 0.52) and total N (r = 0.54). Kinoshita et al. (2012) also observed similar results for CEC (RPD = 2.44), which was strongly correlated with active C (r = 0.86). However, the predictability was moderate for pH and Mg and poor for EC, P, K, Zn, and S, although some of these non-chromophores were strongly correlated with the chromophores in their study. The Pearson correlation is a linear dependency measure based on the assumption of a normal distribution of the correlated attributes. Recently, Kinoshita et al. (2012) reported that no transformations were successful in conforming to a normal distribution for many soil properties in their study. In such situations, the use of r is not advisable. Moreover, the r values are highly sensitive to outliers (Abdullah, 1990). In general, both of these approaches were always not satisfactory in linking covariation with the prediction of all non-chromophores. This necessitates a close examination of the covariation assumption and the dependency measure used in the DRS approach.

In addition to the Pearson correlation coefficient, other dependency measures such as biweight midcorrelation (bicor) and mutual information (MI) are used to account for both linear and nonlinear dependencies (Song et al., 2012). Specifically, these methods have been found to be more robust to outliers than correlation measures. The bicor is a median-based correlation measure, while the MI measures the "distance" between the joint distributions of two variables. The efficacy of such dependency measures has not been explored in soil DRS studies. Thus, the objectives of this study were to: (i) evaluate three dependency measures (r, bicor, and MI) for assessing the covariation of selected non-chromophores with chromophores; and (ii) assess the effects of covariation on the predictability of specific non-chromophores in the DRS approach.

MATERIALS AND METHODS

Study Area and Soil Sampling

This study was conducted using surface (0–10-cm) soil samples from 247 Alfisols and 249 Vertisols collected from different districts of Karnataka, India. The soils were air dried, ground, and sifted through a 2-mm sieve and stored for chemical, physical, and spectral analyses. The soils were collected as a part of a large-scale effort to enhance agricultural productivity across Karnataka State by ICRISAT, Patancheru, Hyderabad, India. These soils were similar to those used by Sarathjith et al. (2014). Alfisols are slightly acidic in reaction because they formed under weathering of ancient crystalline and metamorphic rocks, while the Vertisols are slightly alkaline and are of igneous origin. In contrast to Alfisols, the Vertisols have high base saturation and high soil organic fractions intimately mixed with clay and less dehydrated Fe oxides (Lotse et al., 1972).

Measurement of Soil Properties and Spectral Reflectance

Five chromophores (OC contents, extractable Fe, clay and sand contents, and geometric mean diameter) and seven non-chromophores (pH, EC, P, K, B, Zn, and Al) were estimated for all the soil samples. Soil OC and particle size distribution were determined using the chromic acid digestion method (Walkley and Black, 1934) and the international pipette method (Gee and Bauder, 1986), respectively. Soil pH and EC were measured potentiometrically using a 1:2.5 soil/water ratio. The soil geometric mean diameter (GMD) was determined by dry sieving of 100- to 200-g soil samples in a stack of eight sieves (1.18-, 0.3-, 0.2-, 0.18-, 0.125-, 0.09-, 0.075-, and 0.053-mm nominal diameters) and a pan at the bottom. The samples retained in the top sieve and bottom pan sieve were arbitrarily assigned the aggregate diameter (d_i) of 1.18 and 0.005 mm, respectively. The mass fraction (w_i) of soil aggregates retained in each sieve and the pan were weighed. The GMD was computed as

$$\mathrm{GMD}=\frac{\sum w_i \ln\left(d_i\right)}{\sum w_i} \qquad [2]$$

Extractable P was measured using $NaHCO_3$ as an extractant (Olsen and Sommers, 1982). The NH_4OAc method (Helmke and Sparks, 1996) was used in the estimation of extractable K. Zinc was extracted by diethylenetriaminepentaacetic acid (DTPA) reagent (Lindsay and Norvell, 1978) and B was extracted by hot water (Keren, 1996). Inductively coupled plasma optical emission spectrometry (HD Prodigy, Leeman Labs) was used for nutrient content analysis.

Proximal spectral reflectance of the soil samples at the 350- to 2500-nm range were recorded in the laboratory using a portable spectroradiometer (Field Spec 3 FR, Analytical Spectral Devices Inc.). A contact probe with a 1500-h halogen bulb light source and having 10-mm spot size was used for the active sensing of the soil spectra. About 50 g of soil was placed in an Al moisture box (10-cm diameter) and the soil surface was leveled (Mouazen et al., 2010) with a rubber cork used as a mallet before the spectral measurements. Four reflectance spectra acquired from different quadrants in the central area of the container were smoothed using a third-order Savitsky–Golay filtering algorithm with a span length of 9 nm (Vasques et al., 2010). The average of these four reflectance spectra was calculated to obtain the representative spectrum of the soil. A reference spectrum was collected after every soil sample using a circular (9.2-cm diameter) Spectralon white reference panel (Labsphere).

Relationship of Soil Properties with Spectral Reflectance

All necessary data processing and statistical modeling was performed using MATLAB (R2012a, The Mathworks) software. Soil attributes with a skewed frequency distribution were transformed into natural logarithm or Box–Cox scale. The normality check was performed using the one-sample Kolmogorov–Smirnov test statistic at the 5% significance level. Soil attributes failing the normality test even after logarithmic and Box–Cox transformation were left untransformed. The reflectance values before 400 nm and after 2450 nm were excluded in data modeling due to their poor signal/noise ratio. A range of modeling approaches including the wavelet packet approach (Sahadevan et al., 2013) and partial least squares regression (PLSR) in conjunction several spectral transformations such as absorbance, standard normal variate, Kubelka–Munk, discrete wavelets, and first derivative (FD) were examined in this study. The results of the FD and PLSR combination emerged as the best prediction approach for the majority of the soil attributes in both soil types. Hence, this modeling scheme was adopted for all the soil attributes so as to facilitate model efficacy comparisons across soil attributes.

Outliers in the data sets were removed by analyzing the residuals resulting from the principal component regression relationships between soil property and FD spectra at the 5% level of significance. The remaining soils were partitioned into calibration and validation data sets in a 3:1 ratio by means of the Kennard–Stone algorithm (Kennard and Stone, 1969; Nocita et al., 2014). Relationships between soil attributes and the FD reflectance were established by PLSR. The number of latent variables required for PLSR was determined by a leave-one-out cross-validation scheme (Viscarra Rossel, 2007). The accuracies of the developed PLSR models were evaluated using the coefficient of determination (R^2), root mean squared error (RMSE), and the RPD.

Covariation Assessment Using Dependency Measures

The covariation between the chromophores (X) and a non-chromophore (Y) measured in our study was established by three dependency measures: r, bicor, and MI. The r value indicates the linear dependencies between X and Y, with values bounded between 1 (strong positive correlation) and −1 (strong negative correlation). A value of 0 denotes no correlation between X and Y. If $\bar{X}$ and $\bar{Y}$ denote the average values of X and Y, respectively, for n observations, then r is computed as

$$r(X,Y)=\frac{\sum_{i=1}^{n}(X_i-\bar{X})(Y_i-\bar{Y})}{\sqrt{\sum_{i=1}^{n}(X_i-\bar{X})^2}\sqrt{\sum_{i=1}^{n}(Y_i-\bar{Y})^2}} \qquad [3]$$

The bicor is a median-based correlation measure found to be more robust to outliers than the Pearson correlation (Wilcox, 2005). In this approach, two normalized variables u_i and v_i are first computed using

$$u_i=\frac{X_i-X_{\mathrm{m}}}{9X_{\mathrm{MAD}}} \qquad [4]$$

$$v_i=\frac{Y_i-Y_{\mathrm{m}}}{9Y_{\mathrm{MAD}}} \qquad [5]$$

where X_{m} and Y_{m} represent the medians and X_{MAD} and Y_{MAD} denote the median absolute deviations of X and Y, respectively. The weight for X_i (w_i^X) may then be defined as

$$w_i^X=\left(1-u_i^2\right)I\left(1-\left|u_i\right|\right) \qquad [6]$$

The value of w_i^X ranges between 0 and 1 by assigning the indicator $I(1-|u_i|)$ a value of 1 if $I(1-|u_i|)$ is >0, or 0 otherwise. The weight decreases as X_i moves away from the median and becomes 0 when it exceeds $9X_{\mathrm{MAD}}$. The multiplier 9 in Eq. [4–5] is linked with the scale estimator used in the bicor estimation yielding the optimum efficiency (Wilcox, 2005). A similar weight may be defined for the Y variable (w_i^Y). For the given weights, bicor is then computed as

$$\mathrm{bicor}(X,Y)=\frac{\sum_{i=1}^{n}(X_i-X_{\mathrm{m}})w_i^X(Y_i-Y_{\mathrm{m}})w_i^Y}{\sqrt{\sum_{j=1}^{n}\left[(X_j-X_{\mathrm{m}})w_j^X\right]^2}\sqrt{\sum_{k=1}^{n}\left[(Y_i-Y_{\mathrm{m}})w_i^Y\right]^2}} \qquad [7]$$

Mutual information is a measure of the amount of information that one random variable contains about another random variable. The MI has an added advantage over Pearson correlation in its capacity to measure nonlinear relationships between variables (Battiti, 1994). The MI may be computed as

$$\mathrm{MI}(X,Y)=H(X)+H(Y)-H(X,Y) \qquad [8]$$

where $H(X)$ and $H(Y)$ represent the marginal entropies of X and Y, respectively and $H(X,Y)$ denotes the joint entropy. If $p(x)$ and $p(y)$ are the probability mass functions of X and Y, respectively, and $p(x,y)$ represents their joint distribution, then

$$H(X)=-\sum_{x\in X}p(x)\ln p(x) \qquad [9]$$

$$H(Y)=-\sum_{y\in Y}p(y)\ln p(y) \qquad [10]$$

$$H(X,Y)=-\sum_{x\in X}\sum_{y\in Y}p(x,y)\ln p(x,y) \qquad [11]$$

The MI was computed using the MI toolbox for MATLAB developed by Hanchuan Peng (www.mathworks.in/matlabcentral/fileexchange/14888-mutual-information-computation). The the adjacency values of MI (AMI), which range between 0 and 1, were computed as suggested by Song et al. (2012):

$$\mathrm{AMI}=\frac{2\mathrm{MI}(X,Y)}{H(X)+H(Y)} \qquad [12]$$

RESULTS AND DISCUSSION

Descriptive Statistics of Soil Properties

Descriptive statistics of the different soil properties analyzed in this study are given in Table 1. Generally, Alfisols are dominantly coarse textured and less clayey, in contrast to the Vertisols, which are generally fine-textured and clayey soils. The two soil groups were distinctly different with regard to their clay mineralogy, with the Vertisols being mostly montmorillonitic and the Alfisols being more kaolinitic. The average OC content in both soil types was found to be low and similar in magnitude. The average pH underlined the slight acidic nature of the Alfisols as well as the alkaline nature of the Vertisols.

Reflectance Characteristics of Alfisols and Vertisols

Reflectance spectra for both Alfisols and Vertisols (Fig. 1a) were similar with respect to three distinct absorption peaks around 1400, 1900 (water absorption bands), and 2200 nm (metal–hydroxyl stretching), as reported in the literature (Clark et al., 1990; Post and Noble, 1993). The characteristic absorptions are at montmorillonite singlets (near 1400, 1900, and 2200 nm) in Vertisols and kaolinite doublets (near 1400 and 2200 nm) in Alfisols (Wetterlind and Stenberg, 2010). These two soil groups differed in their overall reflectance. The higher reflectance of Alfisols in the VNIR region may be attributed to their Fe oxide contents (Leone and Sommer, 2000). Moreover, the Vertisols were generally greyish to black in color compared with the more reflective light brown and reddish color of the Alfisol samples. Other spectral dissimilarities between the Vertisols and Alfisols were observed around 550, 850, and 2200 nm (Fig. 1b and 1c). The characteristic feature around 550 and 850 nm may be linked with the electronic transition band of Fe^{2+} and Fe^{3+} (Bayer et al., 2012) in the Alfisols. The absorption peak around 2200-nm wavelength was found to be sharp in the Alfisols and blunt in the Vertisols, which may be associated with the clay mineralogy of these soil types.

Prediction of Soil Properties Using Diffuse Reflectance Spectroscopy

Table 2 lists the regression statistics for the prediction of soil properties of both Vertisols and Alfisols using the FD-PLSR approach with an optimum number of latent variables. Only the extractable Fe and GMD in the Vertisols were accurately predicted among all the soil chromophores in the validation data set. Moderate prediction accuracies were noted for OC in both soil groups and for sand contents, clay contents, and Fe in the Alfisols. The modeling approach failed to estimate sand and clay contents in the Vertisols and GMD in the Alfisols. The pH and P in the Vertisols and the pH and K in the Alfisols were the accurately predicted non-chromophores. Moderate predictions were obtained for EC, Zn, and Al in the Vertisols. Prediction of the remaining soil properties such as K and B in the Vertisols and EC, P, B, Zn, and Al in the Alfisols was poor. The accuracy of prediction calculated in terms of R^2 and the RPD of prediction were comparable and often better than those reported in the literature for extractable Fe (Abdi et al., 2012; Viscarra Rossel and Webster, 2012), clay (Chang et al., 2001; Viscarra Rossel et al., 2006), sand (Kinoshita et al., 2012), OC (Stevens et al., 2006; Morgan et al., 2009; Summers et al., 2011), pH (Malley et al., 1999; Viscarra Rossel and Webster, 2012), EC (Zornoza et al., 2008; Kinoshita et al., 2012), P (Mouazen et al., 2007; Kinoshita et al., 2012; Debaene et al., 2014), K (Volkan Bilgili et al., 2010; Abdi et al., 2012), and Zn (Chang et al., 2001; Kinoshita et al., 2012). Thus, the modeling approach followed in this study may be best suited for these two types of soils.

Table 1. Descriptive statistics of soil properties.

Soil attribute	Vertisols (n = 249)		Alfisols (n = 247)	
	Mean	Range	Mean	Range
Clay, %	14.64 (36)†	4.29–43.42	12.40 (53)	2.10–34.30
Sand, %	65.62 (15)	21.96–87.82	78.10 (10)	50.90–91.60
GMD‡	0.31 (25)	0.17–0.52	0.21 (25)	0.13–0.45
Organic C, %	0.40 (38)	0.11–0.93	0.38 (36)	0.11–0.91
Fe, mg L^{-1}	7.65 (111)	1.20–104.70	14.88 (84)	2.00–104.80
pH	8.54 (6)	6.00–9.60	6.67 (21)	4.30–9.50
EC, μS cm^{-1}	0.58 (318)	0.08–28.20	0.42 (67)	0.10–0.90
P, mg L^{-1}	10.05 (126)	0.47–60.40	11.77 (85)	0.90–57.40
K, mg L^{-1}	232.16 (38)	39.00–618.75	118.83 (89)	11.00–738.00
B, mg L^{-1}	1.59 (105)	0.16–14.72	0.52 (70)	0.10–2.60
Zn, mg L^{-1}	0.65 (161)	0.14–15.24	0.95 (63)	0.22–4.20
Al, mg L^{-1}	1.53 (31)	0.60–4.00	2.23 (53)	1.10–11.20

† Values in parentheses are the coefficients of variation (%).

‡ Geometric mean diameter.

Assessment of Covariation Criteria

Interestingly, not all the chromophores showed excellent predictability; only extractable Fe and GMD in the Vertisols showed excellent prediction, and relatively high RPD values may be seen for OC, Fe, and clay in the Alfisols, although the prediction is only in the moderate range. Table 2 clearly shows that the prediction accuracies for a given non-chromophore are different across soil types. For example, the prediction of K in the Vertisols (RPD = 1.26) and Alfisols (RPD = 2.03) had different strengths of prediction. Some of the non-chromophores showed excellent prediction, however, suggesting that the covariation of a strongly predicted non-chromophore may be linked with the predictability of chromophores. Thus, these two data sets present an opportunity to evaluate the strength of covariation as an indicator of predictability for non-chromophores seen in DRS studies.

Table 3 shows different covariation measures of r, bicor, and AMI for both non-chromophores and chromophores. Although the parameter r does not always indicate causation, the p values ≥99% level of significance indicate strong correlation with chromophores in the Vertisols. Despite significant

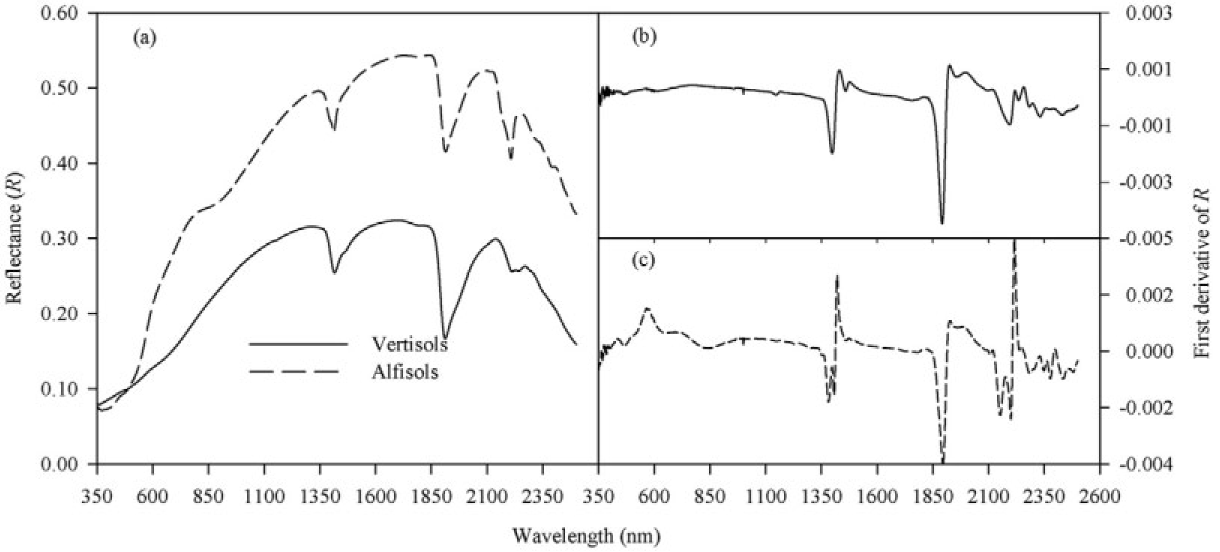

Fig. 1. (a) Average spectral reflectance of Vertisols and Alfisols samples, (b) first derivative of the average reflectance of Vertisols, and (c) first derivative of the average reflectance of Alfisols.

Table 2. Regression statistics of number of latent variables (LV), number of soils (*n*), coefficient of determination (R^2), root mean squared error (RMSE), and residual prediction deviation (RPD) for the prediction of soil properties using diffuse reflectance spectroscopy.

Soil attribute	LV	Calibration			Validation			
		n	R^2	RMSE	*n*	R^2	RMSE	RPD
				Vertisols				
Organic C†	7	175	0.78	0.18	58	0.60	0.19	1.60
Fe‡	9	175	0.91	0.11	59	0.80	0.12	2.24
Clay†	8	176	0.73	0.16	59	0.26	0.20	1.17
Sand	8	178	0.74	4.35	60	0.47	5.87	1.39
GMD§	11	176	0.92	0.02	59	0.84	0.02	2.53
pH¶	9	175	0.89	0.15	58	0.76	0.19	2.07
EC#‡	10	177	0.89	0.43	59	0.56	0.64	1.51
P¶	7	175	0.83	4.07	59	0.80	2.53	2.26
K†	7	175	0.63	0.22	59	0.36	0.20	1.26
B†	14	178	0.91	0.21	59	0.32	0.42	1.23
Zn‡	7	174	0.75	0.34	58	0.57	0.40	1.54
Al‡	10	176	0.78	0.10	59	0.52	0.15	1.46
				Alfisols				
Organic C	8	174	0.72	0.06	58	0.69	0.07	1.82
Fe†	11	175	0.87	0.28	58	0.66	0.40	1.74
Clay†	14	178	0.94	0.13	59	0.69	0.25	1.80
Sand¶	4	174	0.80	3.48	58	0.59	3.50	1.57
GMD†	9	175	0.88	0.09	58	0.43	0.11	1.34
pH¶	11	175	0.92	0.36	58	0.83	0.47	2.46
EC¶	5	176	0.32	0.22	59	0.27	0.22	1.18
P†	9	175	0.54	0.57	59	0.30	0.70	1.20
K†	11	174	0.87	0.28	58	0.75	0.37	2.03
B¶	10	175	0.64	0.18	58	0.39	0.22	1.30
Zn†	9	173	0.66	0.30	58	0.42	0.39	1.32
Al¶	7	179	0.55	0.48	60	0.30	0.44	1.20

† Soil properties subjected to natural logarithm transformation.

‡ Soil properties subjected to Box–Cox transformation.

§ GMD, geometric mean diameter.

¶ Soil properties where transformations failed and data remained untransformed.

EC, electrical conductivity.

correlations with Fe and GMD, which had excellent prediction accuracies (RPD > 2), the parameter EC showed moderate RPD in the Vertisols. In contrast, pH has significant correlation ($p < 0.001$) with all the chromophores except GMD and showed excellent predictability (RPD > 2) for this soil group. Such an inconsistent trend for Pearson correlation precludes its use as a good dependency measure for explaining covariation and its role in the estimation of non-chromophores in the DRS approach.

Except for a few isolated cases, bicor showed similar trends as the r values. This was expected because bicor and r values should be similar for most normally distributed data and we had most of our parameters transformed to have a normal distribution. Similar to r values, MI also did not explain the excellent prediction for pH and moderate prediction for EC despite large adjacency values. With the lack of a test of significance, the superiority of AMI factors could not be assessed, although their range appeared to be narrow compared with the two other dependency measures: AMI values ranged from 0.01 to 0.34 and r values ranged from −0.81 to 0.65. With no one-to-one relationship between the dependency measures and the RPD values, we also examined whether these measures as a group could explain the strength of prediction as influenced by the strength of dependency. We estimated an average dependency index (ADI) by taking the average of the absolute dependency values shown in Table 3 for all the chromophores (OC, sand, clay, Fe, and GMD) for each non-chromophore with the assumption that the covariation assessment may be more appropriate when the dependencies (significant or insignificant) of a non-chromophore with several chromophores are considered together rather than examining them for individual chromophores. Thus, three ADI values corresponding to r (ADI_r), bicor ($\mathrm{ADI}_{\mathrm{bicor}}$) and AMI ($\mathrm{ADI}_{\mathrm{AMI}}$) were estimated for each non-chromophore. Figures 2a, 2b, and 2c show these three ADI values as functions of the corresponding RPD values for all seven non-chromophores considered for both the soil groups. A linear trend between the RPD values and ADI_r ($R^2 = 0.39$), $\mathrm{ADI}_{\mathrm{bicor}}$ ($R^2 = 0.37$) and $\mathrm{ADI}_{\mathrm{AMI}}$ ($R^2 = 0.49$) values may be noted, suggesting that the increase in the predictability of a non-chromophore is tied with how strongly it depends on all the chromophores and not just one of them.

To further assess the linearity between the ADI and RPD values, we further estimated the ADI values corresponding to physical (clay, sand, GMD) and chemical (OC and Fe) chromophores separately. Many soil DRS studies explained the prediction of a non-chromophore by its covariation with physical, chemical, or a combination of both (combined chromophores) categories. Recently, both Abdi et al. (2012) and Nduwamungu et al. (2009) linked the prediction of pH with total C and total N (chemical chromophores). Chang et al. (2001) reported that the prediction of pH was dependent on clay and organic matter (combined chromophores). The ADI values for the physical chromophores (Fig. 2d–2f) show no linear association between the RPD values and ADI_r ($R^2 = 0.00$), $\mathrm{ADI}_{\mathrm{bicor}}$ ($R^2 = 0.00$), and $\mathrm{ADI}_{\mathrm{AMI}}$ ($R^2 = 0.00$), suggesting that the physical chromophores may be least significant in explaining the predictability of non-chromophores despite the strong dependencies that existed between them. The reason may be associated with the lack of absorption at discrete wavelengths in the reflectance spectra for physical chromophores. In contrast, the influence of chemical chromophores at discrete wavelengths in the spectra together with their dependency for non-chromophores may have resulted in a very strong linear relationship between the RPD values of the non-chromophores and ADI_r ($R^2 = 0.73$), $\mathrm{ADI}_{\mathrm{bicor}}$ ($R^2 = 0.77$), and $\mathrm{ADI}_{\mathrm{AMI}}$ ($R^2 = 0.93$) values (Fig. 2g–2h). The performances of ADI_r, $\mathrm{ADI}_{\mathrm{bicor}}$, and $\mathrm{ADI}_{\mathrm{AMI}}$ were superior when only chemical chromophores were considered in their computation. All the non-chromophores considered in this study are generally chemical in nature. This suggests that the prediction of

Table 3. Covariation between non-chromophores and chromophores.

Chromophore	Vertisols							Alfisols						
	pH	EC†	P	K	B	Zn	Al	pH	EC	P	K	B	Zn	Al
Pearson correlation coefficient														
Organic C	−0.32**	0.14	0.49**	0.28**	0.03	0.36**	−0.01	0.39**	−0.20*	0.21**	0.65**	0.29**	0.39**	−0.19*
Fe	−0.24**	0.26**	0.63**	−0.17*	0.12	0.43**	−0.21*	−0.81**	0.20*	0.10	−0.55**	−0.12	−0.15	0.03
Clay	0.24**	0.45**	0.18*	0.08	0.48**	0.19*	−0.24**	−0.45**	0.19*	−0.19*	−0.44**	0.04	−0.33**	−0.12
Sand	−0.35**	−0.54**	−0.06	−0.17*	−0.60**	−0.14	0.32**	0.01	−0.02	0.16	0.04	−0.20*	0.21**	0.18*
GMD‡	−0.06	0.55**	0.42**	0.03	0.49**	0.45**	−0.15	−0.11	0.06	−0.18*	−0.19*	0.06	−0.28**	0.03
Biweight midcorrelation														
Organic C	0.41	0.13	0.49	0.29	0.03	0.36	0.04	0.41	0.18	0.20	0.66	0.26	0.42	0.19
Fe	0.24	0.28	0.59	0.14	0.15	0.46	0.22	0.82	0.19	0.10	0.56	0.06	0.15	0.06
Clay	0.23	0.48	0.2	0.08	0.50	0.21	0.19	0.48	0.16	0.16	0.45	0.02	0.35	0.29
Sand	0.28	0.53	0.07	0.16	0.57	0.12	0.28	0.00	0.08	0.15	0.03	0.16	0.16	0.34
GMD	0.08	0.56	0.4	0.01	0.50	0.45	0.15	0.11	0.08	0.18	0.19	0.03	0.26	0.15
Mutual information based adjacency values														
Organic C	0.17	0.05	0.13	0.10	0.08	0.07	0.07	0.09	0.08	0.05	0.17	0.12	0.09	0.05
Fe	0.13	0.14	0.28	0.07	0.10	0.12	0.07	0.34	0.06	0.09	0.13	0.06	0.06	0.11
Clay	0.12	0.14	0.04	0.06	0.16	0.06	0.09	0.18	0.03	0.08	0.13	0.05	0.08	0.13
Sand	0.12	0.13	0.03	0.10	0.18	0.07	0.10	0.04	0.01	0.05	0.04	0.07	0.07	0.08
GMD	0.07	0.13	0.11	0.05	0.14	0.10	0.04	0.05	0.02	0.05	0.04	0.07	0.05	0.07

* Significant at $p < 0.01$.

** Significant at $p < 0.001$.

† EC, electrical conductivity.

‡ GMD, geometric mean diameter.

chemical non-chromophores was mainly due to their dependencies with the chemical chromophores.

A similarity in the spread of data points may also be noted in the scatter diagrams for ADI_r and $\mathrm{ADI}_{\mathrm{bicor}}$. This may due to the fact that the dependency measures based on the mean (r) and median (bicor) look similar when the variables are normally distributed. In this study, most of the soil properties were transformed to have normality in their frequency distribution. Interestingly, the $\mathrm{ADI}_{\mathrm{AMI}}$ outperformed ADI_r and $\mathrm{ADI}_{\mathrm{bicor}}$ in case of combined physical and chemical chromophores. The capability of AMI to account for nonlinearities associated with some of the untransformed soil attributes may have resulted in the better performance of $\mathrm{ADI}_{\mathrm{AMI}}$ (Fig. 2c, 2f, and 2i). The strong linkage between the RPD and $\mathrm{ADI}_{\mathrm{AMI}}$ values was well depicted when the latter was computed using the chemical chromophores alone (Fig. 2i). Almost all the data points were located very close to the best-fit line ($R^2 = 0.93$) in the scatter diagram. Moreover, the slope of the regression lines between RPD and $\mathrm{ADI}_{\mathrm{AMI}}$ was more than those of the other two dependency measures, suggesting higher sensitivity of the MI measure for the predictability. Similarly, the intercept of the RPD vs. $\mathrm{ADI}_{\mathrm{bicor}}$ regression line was larger than the other two dependency measures, suggesting greater dependency of RPD on $\mathrm{ADI}_{\mathrm{bicor}}$; however, the R^2 for the regression line was less compared with the $\mathrm{ADI}_{\mathrm{AMI}}$. Thus, the excellent relationship found between the RPD and $\mathrm{ADI}_{\mathrm{AMI}}$ suggests that the prediction of the non-chromophores in the study may be related to their AMI with the chemical chromophores. Thus, the use of AMI may be advocated as a better covariation measure capable of explaining the predictability of non-chromophores in DRS studies.

SUMMARY AND CONCLUSIONS

The prediction of non-chromophores using the DRS approach is assumed to be related to their covariation with chromophores, but none of the existing methods and analyses succinctly depicts the linkage between covariation measures and the predictability of a non-chromophore. This study was performed to find an appropriate dependency measure to evaluate the covariation assumption using two major soil groups of India. Based on the fundamental definition of chromophores, OC and Fe were considered as chemical chromophores, soil texture and GMD as physical chromophores. The other soil properties, namely pH, EC, P, K, B, Zn, and Al, were treated as non-chromophores. The first derivative of soil reflectance in conjunction with the PLSR modeling approach was used for predicting all the soil properties. The model accuracies were evaluated using RPD. The utility of three different dependency measures, namely r, bicor, and AMI, were examined. An overall covariation measure was generated for each dependency measure (ADI_r, $\mathrm{ADI}_{\mathrm{bicor}}$, and $\mathrm{ADI}_{\mathrm{AMI}}$) as the average of the dependency values of a non-chromophore with different chromophores. The covariation assessment was performed for three chromophore groups (combined, physical, and chemical). Linkage between the RPD of non-chromophores and ADI_r, $\mathrm{ADI}_{\mathrm{bicor}}$, and $\mathrm{ADI}_{\mathrm{AMI}}$ was examined for each chromophore group. It was noted that the predictability of non-chromophores was mainly due to their dependency with chemical chromophores. The physical and combined chromophores were less reliable for explaining the predictability of non-chromophores with any of the dependency indices. Among the three dependency indices, the performance of $\mathrm{ADI}_{\mathrm{AMI}}$ was superior to ADI_r and $\mathrm{ADI}_{\mathrm{bicor}}$. An excellent relationship ($R^2 = 0.93$)

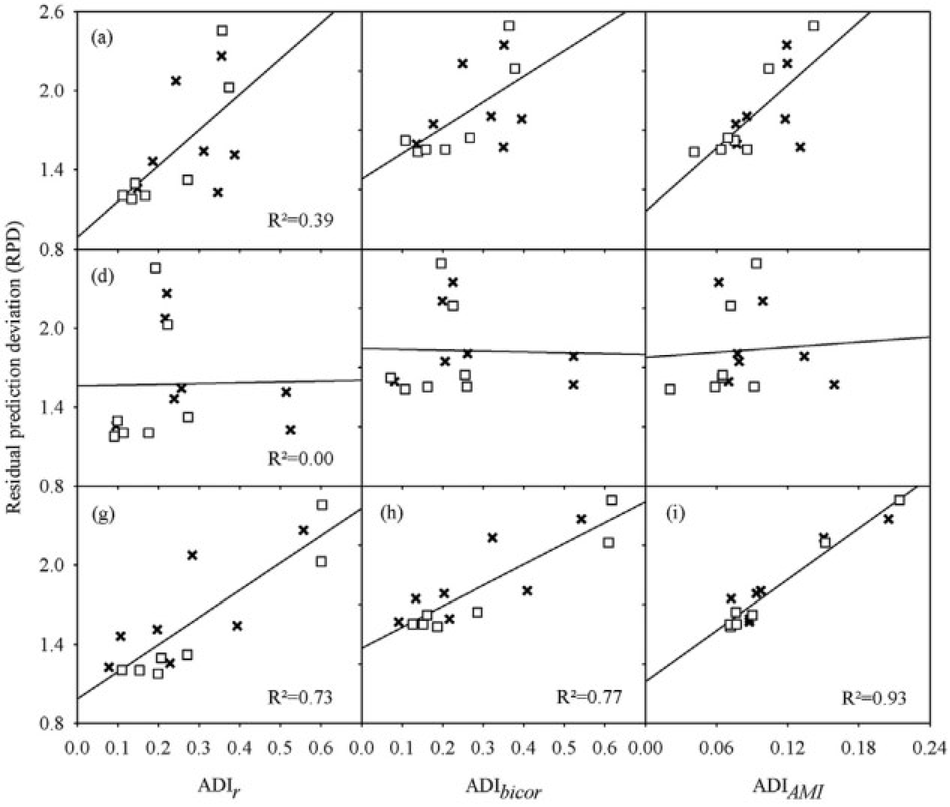

Fig. 2. Linkage between the average dependency index (ADI) of the Pearson correlation coefficient (*r*), the biweight midcorrelation (bicor), and the mutual information based adjacency values (AMI) and the residual prediction deviation (RPD) of non-chromophores.

between RPD and ADI$_{\text{AMI}}$ was found in the case of chemical chromophores. This implies that the prediction of a non-chromophore relies on its AMI with chemical chromophores. Thus, the use of AMI may be advocated rather than the conventional use of *r* for evaluating the covariation between chromophores and non-chromophores.

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