SPECTRAL CHARACTERIZATION OF ALFISOLS AND VERTISOLS BY DIFFUSE REFLECTANCE SPECTROSCOPY

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SPECTRAL CHARACTERIZATION OF ALFISOLS AND VERTISOLS BY DIFFUSE REFLECTANCE SPECTROSCOPY

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by

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Under the guidance of

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- **M. C. Sarathjith**, B. S. Das, S. P. Wani, and K. L. Sahrawat. 2014. Dependency Measures for Assessing the Co-variation of Spectrally-Active and Spectrally-Inactive Soil Properties in Diffuse Reflectance Spectroscopy, Soil Sci. Soc. Am. J. (*In review*).

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Signature

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ABBREVIATIONS

ABS	Absorbance
ADI	Average Dependency Index
AIC	Akaike Information Criterion
AMI	Adjacency Values of Mutual Information
ANN	Artificial Neural Networks
ASD	Aggregate Size Distribution
bicor	Biweight Midcorrelation
CEC	Cation Exchange Capacity
CR	Continuum Removal
CT	Committee Trees
CV	Coefficient of Variation
DRS	Diffuse Reflectance Spectroscopy
DT	Detrending
DTPA	Diethylene Triamine Penta-Acetic Acid
DWT	Discrete Wavelet Transform
EC	Electrical Conductivity
EMR	Electromagnetic Radiation
ET	Electronic Transitions
FD	First Derivative
GMD	Geometric Mean Diameter
ICP-OES	Inductively Coupled Plasma Optical Emission Spectrometry
ICRAF	International Centre For Research In Agroforestry
ICRISAT	International Crops Research Institute For Semi-Arid Tropics
IR	Infrared
ISRIC	International Soil Reference And Information Centre
IUSS	International Union Of Soil Sciences
KM	Kubelka-Munk
KS	Kolmogorov-Smirnov

LOOCV	Leave-One-Out Cross Validation
LUCAS	Land Use/Cover Area Frame Statistical Survey
MARS	Multivariate Adaptive Regression Splines
MATLAB	Matrix Laboratory
max	Maximum
MaxN	Maximum Normalization
MC	Mean Centering
MeanN	Mean Normalization
MI	Mutual Information
min	Minimum
MIR	Mid-Infrared
MLR	Multiple Linear Regression
MRA	Multi Resolution Analysis
MSC	Multiplicative Scatter Correction
MSE	Mean-Squared-Error
MWD	Mean Weight Diameter
NER	Noise Equivalent Radiance
NIR	Near–Infrared
OC	Organic Carbon
OM	Organic Matter
PCR	Principal Component Regression
PLSR	Partial Least Square Regression
PTF	Pedotransfer Functions
R	Reflectance
RCO	Residual Case Order
RER	Ratio Error Range
RMSE	Root Mean Squared Error
RPD	Residual Prediction Deviation
RPIQ	Ratio of Performance to Inter-Quartile Distance
RT	Regression Tree

SD	Second Derivative
SEC	Standard Error of Calibration
SEP	Standard Error of Prediction
SG	Savitzky–Golay Smoothing
SMLR	Stepwise Multiple Linear Regression
SNV	Standard Normal Variate
SS	Smooth Spline
STF	Spectrotransfer Functions
SWIR	Shortwave–Infrared
TE	Thermoelectric
U.S.	United States
UT	Untransformed
UV	Ultraviolet
VIP	Variable Importance for Projection
VIS	Visible
VN	Vector Normalization
VNIR	Visible-Near-Infrared

SYMBOLS

$\bar{X}$	:	Mean of variable X
$\bar{Y}$	:	Mean of variable Y
$\hat{Y}$	:	Predicted soil property
$\bar{Y}$	:	Mean of observed soil property
w_{jk}^2	:	Loading weight of the k^{th} variable in the j^{th} PLSR factor
$\hat{y}$	:	Box-Cox power transformed soil property
μ_R	:	Mean of reflectance
a	:	Scattering coefficient/ Number of factors
b	:	Offset
d	:	Aggregate diameter (mm)
d_m	:	Mean aggregate diameter
e	:	Soil constituent information
$erfc$	:	Complementary error function
f	:	Frequency distribution
$H(X)$	:	Marginal entropy of X
$H(X,Y)$	:	Joint entropy of X and Y
$H(Y)$	:	Marginal entropy of Y
I	:	Indicator
K	:	Total number of predictor variables
ln	:	Natural logarithm
LV	:	Number of latent variables
n	:	Number of observations or soil samples
p	:	Level of significance
$p(x)$	:	Probability mass function of X
$p(x,y)$	:	Joint probability distribution of X and Y
$p(y)$	:	Probability mass function of Y
Q_1	:	First quartile of soil property

Q_3	:	Third quartile of soil property
R	:	Reflectance spectrum
r	:	Pearson correlation coefficient
R^2	:	Coefficient of determination
R_{ref}	:	Reference spectrum
SSY_j	:	Explained sum of squares of soil property
SSY_t	:	Total sum of squares of soil property
u_i	:	Normalized variable of X
v_i	:	Normalized variable of Y
W	:	Cumulative aggregate mass fraction
w_i	:	Mass fraction of soil aggregates (g)
w_i^X	:	Weight for X
w_i^Y	:	Weight for Y
X	:	A variable
X_m	:	Median of X
X_{mad}	:	Median absolute deviation of X
Y	:	Observed soil property
y	:	Soil property
Y	:	A variable
Y_i	:	Observed response variable
Y_m	:	Median of Y
Y_{mad}	:	Median absolute deviation of Y
β	:	Regression coefficient
δ	:	Bending mode
λ	:	Wavelength/ Box-Cox parameter
v	:	Overtone
σ	:	Standard deviation of aggregate size distribution function
σ_R	:	Standard deviation of reflectance

ABSTRACT

Rapid assessment of soil characteristics is pre-requisite for the management of agricultural resources. Over the last two decades, diffuse reflectance spectroscopy (DRS) is emerging as a promising technology for the rapid assessment of several soil properties. A prerequisite in the DRS approach is the availability of robust relationships between soil properties and corresponding reflectance spectra. Generally, large databases on soil properties and soil reflectance spectra are required to develop such spectral algorithms. Review of the DRS studies revealed that only a limited effort has been made to apply the DRS approach to Indian soils and the performance of the DRS approach is often not satisfactory especially in low carbon soils. In this study, spectral algorithms were developed for estimating both chromophores (organic carbon; texture; iron content; aggregate size distribution, ASD characteristics) and non-chromophores (pH, electrical conductivity, phosphorus, potassium, sulfur, boron, zinc, aluminum) in two major soil orders Alfisols and Vertisols of Karnataka state in India. Partial least squares regression models were used to develop spectral algorithms. Model accuracy was evaluated using residual prediction deviation (RPD). The DRS approach yielded mixed results in predicting basic soil properties and nutrient contents. The first derivative-based DRS models yielded accurate prediction of most of ASD characteristics in both the soil types. The co-variation assumption was also evaluated using three dependency measures (Pearson correlation coefficient, *r*; biweight midcorrelation, *bicor*; and adjacency values of mutual information, AMI) by generating an average dependency index (ADI) for each of the three measures (ADI_r, ADI_{bicor} and ADI_{AMI}). The relationships between RPD values of non-chromophores and the ADI values were ascertained for different chromophore groups (physical, chemical and combined). The ADI_{AMI} outperformed ADI_r and ADI_{bicor}. The ADI_{AMI} computed using chemical chromophores showed strong linear relationships ($R^2 = 0.93$) between ADI_{AMI} and RPD of chemical non-chromophores suggesting that the AMI may be used as a robust dependency measure to assess the co-variation of non-chromophores with chromophores. The study demonstrated the use of DRS approach in the characterization of low carbon soils, prediction of ASD characteristics and a MI based dependency measure for 'co-variation' assessment.

Keywords: diffuse reflectance spectroscopy, aggregate size distribution, chromophores, non-chromophores, organic carbon, partial least squares regression, residual prediction deviation, Pearson correlation coefficient, biweight midcorrelation, mutual information.