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Gan-Lin Zhang
Dick Brus
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Editors
Gan-Lin Zhang
Institute of Soil Science
Chinese Academy of Sciences
Nanjing
China

Xiao-Dong Song
Institute of Soil Science
Chinese Academy of Sciences
Nanjing
China

Dick Brus
Soil Science
Alterra
Wageningen
The Netherlands

Philippe Lagacherie
National Institute for Agricultural Research
Paris
France

Feng Liu
Institute of Soil Science
Chinese Academy of Sciences
Nanjing
China

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Chapter 21
Transferability and Scaling of VNIR Prediction Models for Soil Total Carbon in Florida

Congrong Yu, Sabine Grunwald and Xiong Xiong

Abstract The assessment of soil total carbon (TC) across large land areas is critical to derive global and regional soil carbon budgets and better understand the interactions between carbon and other biogeochemical cycles. But the cost and time involved in measurements of TC with standard laboratory methods are impractical. Research has suggested that visible/near-infrared (VNIR) diffuse reflectance spectroscopy can provide robust and accurate estimations for TC. The applicability, transfer, and scalability of VNIR-derived soil models are still poorly understood. The objectives of this study in Florida, USA, were to (i) compare two methods to predict soil TC using five fields (local scale) and a pooled (regional scale) VNIR spectral dataset, (ii) assess the model's transferability among fields, and (iii) evaluate the up- and downscaling behavior of TC prediction models. A total of 560 TC-spectral sets were modeled by partial least squares regression (PLSR) and support vector machine (SVM). The transferability and up- and downscaling of models were limited by the following factors: (i) the spectral data domain, (ii) soil attribute domain, (iii) methods that describe the internal model structure of VNIR-TC relationships, and (iv) environmental domain space of attributes that control soil carbon dynamics. All soil logTC models showed excellent performance based on both methods (PLSR and SVM) with $R^2 > 0.86$, bias < 0.01 %, root-mean-square prediction error (RMSE) = 0.09 %, residual predication deviation (RPD) > 2.70 %, and ratio of prediction error to inter-quartile range (RPIQ) > 4.54. PLSR performed substantially better than SVM to scale and transfer models. Upscaled soil TC models performed somewhat better in terms of model fit (R^2), RPD, and RPIQ, whereas downscaled models showed less bias and smaller RMSE based on PLSR. But no universal trend was found indicating which of the four investigated factors (i–iv) had the most impact that constraints transferability and scalability. The findings from this study have implications for the development of

C. Yu · S. Grunwald (✉) · X. Xiong
Department of Soil and Water Science, University of Florida, Gainesville, USA
e-mail: sabgru@ufl.edu

C. Yu
State Key Lab of Hydrology-Water Resources and Hydraulic Engineering,
College of Hydrology and Water Resource, Hohai University, Nanjing, Jiangsu, China

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'universal' spectral-based soil models aiming to predict soil properties for a diverse set of different soils formed in different environmental conditions covering a wide range of geographic settings, at its extreme the whole globe. Those 'universal' spectral libraries are based on the premise that soil predictions (e.g., soil TC) can be made anyplace because they are built using soil spectral datasets that characterize exhaustively the attribute feature space. This assertion is limited by the fact that a large number of interacting factors of soils, spectra, and environmental properties are needed to represent the exhaustive sample population which has not materialized yet. Given the many factors that can impinge on empirically derived soil spectral prediction models, as demonstrated by this study, more focus on the applicability and scaling of them is needed.

Keywords Soil organic carbon · Visible/near-infrared spectroscopy · Transferability · Scalability · Modeling

21.1 Introduction

Research has suggested that visible/near-infrared (VNIR) diffuse reflectance spectroscopy can provide robust and accurate estimations for TC and carbon fractions (Viscarra Rossel et al. 2006; Vasques et al. 2009, 2010; Nocita et al. 2011; Sarkhot et al. 2011; McDowell et al. 2012a, b). Spectral soil carbon models are poised to contribute to spatially explicit regional and global carbon assessment. However, knowledge gaps still exist in terms of the prediction quality across different soils and landscapes, transferability, and scalability of such models. Scaling and transfer concepts and their implications for modeling were presented by Blöschl and Sivapalan (1995), Wu et al. (2006), and Grunwald et al. (2011).

Given the multitude of potential factors that may impact the application of VNIR soil carbon models to make predictions for unknown samples, the underlying motivation for this research was to design an experimental study to investigate the transfer and up- and downscaling behavior of soil TC-VNIR models. The specific objectives were to (i) compare the performance of two methods to predict soil TC using five fields (local) and a pooled (regional) VNIR spectral dataset, (ii) assess the model's transferability among five representative field sites in Florida, (iii) evaluate the upscaling and downscaling behavior of TC prediction models, and (iv) examine the constraining factors in model transferability and scaling.

21.2 Data and Methods

Five fields (each of size ~ 0.25 km^2) were selected that represent prominent soil–land-use types in Florida, USA (Xiong 2013). Table 21.1 provides a description of the main landscape characteristics of each field. A total of 112 samples (0–20 cm depth)

Table 21.1 Characteristics of the five fields

	Variables	Study areas				
		Field 1	Field 2	Field 3	Field 4	Field 5
	Sampling location	Ordway-Swisher Biological Station	San Felasco Hammock Preserve State Park	Econfina Creek Water Management area	Santa Fe River Ranch	Myakka River State Park
	Longitude	81° 59′9″W	82° 27′31″W	85° 33′51″W	82° 29′40″W	82° 17′16″W
	Latitude	29° 41′23″N	29° 43′59″N	30° 26′42″N	29° 55′45″N	27° 11′22″N
Topography	Elevation (m)[a]	42.8	43.5	23.9	28.8	8.7
	Slope (%)[a]	1.2	1.2	2.9	2.4	0.2
Climate	Max temperature (°C)[b]	27.5	27.1	26.3	27.2	29.2
	Min temperature (°C)[b]	14.0	13.8	12.9	13.6	16.3
	Precipitation (mm)[b]	1325	1345	1634	1360	1464
Parent material	Surficial geology[c]	Cypresshead	Coosawhatchie	Citronelle	Coosawhatchie	Shelly sediments of plio-pleistocene
Organism	Land use	Xeric upland forest	Mesic upland forest	Pineland	Improved pasture	Rangeland
	NPP (kg C m^{-2})[d]	7.91	13.60	9.07	7.50	8.13
	NDVI[d]	3.81	7.90	3.81	9.50	4.31
	Dry biomass (kg m^{-2})[e]	2.76	12.50	5.53	–	6.68
Soil	Soil suborder[f]	Psamments	Aquults-psamments-udepts-udults	Psamments	Udults	Aquods
	AWC (cm cm^{-1})[f]	1.2	2.1	1.5	2.2	1.7
	Clay content (%)[f]	1.2	5.2	3.7	4.6	1.9
	Sand content (%)[f]	98.6	93.2	93.1	90.8	96.8

Variable descriptions, abbreviations, and sources

[a]National Elevation Dataset (NED), United States Geological Survey (USGS) (1999)

[b]Long-term maximum and minimum annual average temperature, long-term annual average precipitation between 1971 and 2000 from Parameter-elevation Regressions on Independent Slopes Model (PRISM) climate group

[c]USGS 1998; Florida Fish and Wildlife Conservation Commission (2003)

[d]Net primary productivity (NPP), normalized difference vegetation index (NDVI) from Moderate-Resolution Imaging Spectroradiometer (MODIS) for North American Carbon Project 2005

[e]National Biomass and Carbon Dataset (NBCD) 2000

[f]Soil suborder, available water holding capacity at 0–25 cm (AWC), clay content and sand content at 0–20 cm from Soil Survey Geographic Database (SSURGO), Natural Resources Conservation Service (NRCS) (2009)

in each field were collected (whole dataset comprising five fields $n = 560$) using the unbalanced nested spatial sampling design described by Lark (2011). In each field, at first, nine main centers gridded at 200-m intervals were chosen to constitute the highest level of the hierarchy. Secondly, at each main center, one additional sampling point (subnode) was collected 67 m away in a random direction. In similar pattern, the 2nd, 3rd, and 4th hierarchical sampling points were fixed at locations 22, 7, and 2 m away from their parent nodes, respectively. The approximately threefold hierarchy has been proven to be effective in capturing soil variation and avoiding overlaps among different branches (Webster and Oliver 2007).

Soil TC content was measured by dry combustion in the laboratory using a Shimadzu TOC-5050 analyzer (Table 21.2). The samples were 2 mm sieved and then oven dried at 40–45 °C for 12 h before scanning with a QualitySpec Pro Spectroradiometer (Analytical Spectral Devices Inc., Boulder, CO) in the VNIR spectral range (350–2500 nm) with a 1-nm-interval spectral resolution. For each sample, four replicate scans were taken at each of the four quadrants of a petri dish by rotating the sample at angles of 90°. The spectrometer was recalibrated to remove the baseline at every 10 samples with white spectralon. An average reflectance spectral curve was obtained for each sample that was used for modeling. Two preprocessing transformations were applied to the soil reflectance curves: First, the reflectance curves were smoothed across a moving window of nine nm using the Savitzky–Golay algorithm with a third-order polynomial to reduce the random noise (Savitzky and Golay 1964). Second, the first-degree Savitzky–Golay derivative with a search window of seven measurements and second-order polynomial was applied to the smoothed curves.

Two different multivariate regression techniques were applied to develop spectral models to predict logTC: partial least squares regression (PLSR) (Martens and Næs 1989) and support vector machine (SVM) (Vapnik 2000). First, leave-one-out

Table 21.2 Descriptive statistics of measured soil total carbon (original values: TC, logarithm-transformed values: logTC)

		TC (%)						logTC (log %)			
Datasets	*n*	Min.	Median	Mean	Max.	CV	Skew.	Mean	SD	CV	Skew.
Whole	560	0.31	1.04	1.18	3.55	0.55	0.99	0.01	0.24	30.56	0.06
Field 1	112	0.32	0.56	0.59	1.12	0.28	1.02	−0.24	0.11	−0.47	0.37
Field 2	112	0.70	1.63	1.77	3.35	0.36	0.78	0.22	0.15	0.68	0.15
Field 3	112	0.31	0.62	0.68	2.32	0.42	3.28	−0.20	0.14	−0.70	1.28
Field 4	112	0.56	1.05	1.10	2.84	0.30	2.25	0.030	0.11	4.48	0.74
Field 5	112	1.02	1.69	1.76	3.55	0.26	0.80	0.23	0.11	0.47	0.09
CAL	392	0.33	1.02	1.17	3.55	0.55	1.06	0.01	0.23	31.77	0.11
VAL	168	0.31	1.07	1.19	3.21	0.55	0.86	0.01	0.24	28.53	−0.02
SUB-W	112	0.32	1.04	1.20	2.85	0.53	0.69	0.02	0.24	15.29	−0.04

CAL = the dataset used to calibrate the models; VAL = the dataset used to validate the models; SUB-W = the 112 observations randomly chosen from the five fields (Fig. 21.1); *n* = number of observations; SD = standard deviation; CV = coefficient of variation; skew. = skewness

(LOO) cross-validation was employed to evaluate the model performance of the CAL datasets (70 % or $n = 392$ of the whole dataset). Second, independent validation was used to assess the model performance using the VAL datasets (30 % or $n = 168$ of the whole dataset). The coefficient of determination (R^2) was used as the goodness-of-fit statistic. The root-mean-square error (RMSE), residual prediction deviation (RPD) (Williams 1987), ratio of performance to inter-quartile distance (RPIQ) (Bellon-Maurel et al. 2010), and bias (Davies and Fearn 2006) were provided as complementary error statistics to evaluate the performances of different prediction models.

The transferability and scalability analyses were conducted using PLSR and SVM models. In this study, the definitions of 'model transfer,' 'scale transformation,' and 'up-/downscaling' as provided by Blöschl and Sivapalan (1995) and Wu et al. (2006) were adopted. Hence, 'transferability' denotes the transfer (or application) of a VNIR-based soil TC prediction model (Models 1 to 5) developed at one field site (Fields 1, 2, 3, 4, and 5, respectively) to another field site (Fields 1, 2, 3, 4, and 5, respectively) (Fig. 21.1b). The model performance at calibration sites was assessed using LOO cross-validation, and transferability was assessed using R^2, RMSE, RPD, and RPIQ. In this paper, 'scalability' denotes a change in the extent (size) of the geographic area represented by models, 'upscaling' refers to an escalation of the area (i.e., from smaller to larger extent), and 'downscaling' refers to the contraction of the area (i.e., from larger to smaller extent) Wu et al. 2006) (Fig. 21.1c, d). In the scaling analysis, a pooled subset-whole (SUB-W) dataset was created ($n = 112$) randomly selected from the whole dataset ($n = 560$) (Fig. 21.1a). The observation size of the SUB-W was equal to that of each field ($n = 112$),

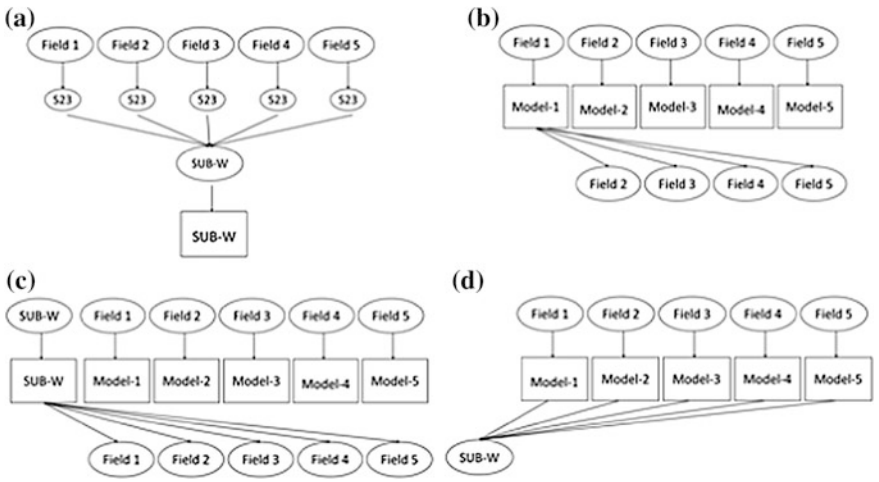

Fig. 21.1 The principle scheme of the transferability and scaling analysis: **a** the sample source of SUB-W dataset; **b** transferability at field scale; **c** downscaling analysis; **d** upscaling analysis. *Note* S23 in Fig. 21.1a represented the 23 samples randomly chosen from each of the five fields to calibrate the regional model

eliminating any bias or negative effects caused by the different sample sizes on the comparative analysis. To assess the downscaling behavior, the regional SUB-W models were applied to each of the five fields (Fig. 21.1c). And vice versa, to assess the upscaling performance, the TC models using PLSR and SVM developed for each of the five fields were applied to the regional SUB-W dataset (Fig. 21.1d). The same error statistics as outlined above were used to evaluate scaling behavior of TC models.

The Gower similarity coefficient (Gower 1971), as outlined in Mallavan et al. (2010), was employed to measure the similarity in soil-forming factors among fields according to Eq. (21.1). Important variables that were included in the similarity analysis are shown in Table 21.1.

$$S_{ij} = \frac{1}{p}\sum_{k=1}^{p}\left(1 - \frac{\left|x_{ik} - x_{jk}\right|}{\text{range } k}\right) \tag{21.1}$$

where S_{ij} is the Gower similarity coefficient between two sites i and j; k represents the soil-forming factors (i.e., environmental covariates); p is the number of variables; range k is the value range of variable k in the whole study area.

21.3 Results and Discussion

21.3.1 Prediction Performance of Spectral Prediction Models

The TC predictions derived from PLSR and SVM across all five fields (Table 21.3) and at the five field sites (Table 21.4) showed moderate performance. The R^2 was ≥0.86, and the RPIQ ≥4.54 for the whole dataset (Table 21.3). Brown et al. (2005) found that VNIR models developed using boosted regression trees (BRTs) outperformed PLSR to predict soil organic carbon (SOC) and soil TC, while McDowell

Table 21.3 Summary statistics for the spectral models of logTC produced by partial least squares regression (PLSR) and support vector machine (SVM) derived from calibration (CAL) using 70 % of all the samples (n = 392) and validation using 30 % of the samples (n = 168)

	LOO cross-validation using CAL		Validation using VAL				
	R^2	RMSE (log %)	R^2	Bias (log %)	RMSE (log %)	RPD	RPIQ
PLSR	0.88	0.08	0.86	0.004	0.09	2.70	4.54
SVM	0.87	0.09	0.88	0.01	0.09	2.78	4.67

LOO cross-validation = leave-one-out cross-validation; R^2 = coefficient of determination; RMSE = root-mean-squared deviations; RPD = residual prediction deviation; RPIQ = ratio of prediction error to inter-quartile range

Table 21.4 Summary statistics of leave-one-out cross-validation for partial least squares regression (PLSR) and support vector machine (SVM) models of logTC (log %) developed in SUB-W and the five field datasets

Models	PLSR		SVM	
	R^2	RMSE (log %)	R^2	RMSE (log %)
Model SUB-W	0.82	0.10	0.84	0.10
Model 1	0.69	0.06	0.55	0.08
Model 2	0.62	0.10	0.59	0.11
Model 3	0.46	0.10	0.33	0.11
Model 4	0.56	0.07	0.59	0.08
Model 5	0.61	0.07	0.52	0.08

R^2 = coefficient of determination; RMSE = root-mean-squared deviations; SUB-W = the 112 observations randomly chosen from the five fields (Fig. 21.1)

et al. (2012b) found no significant difference among PLSR and random forest (RF) ensemble regression trees to predict soil TC on Hawaiian soils. Minasny and McBratney (2008) and Minasny et al. (2009) in Australia found excellent predictions for SOC and TC using regression rules (Cubist approach). In contrast, Vasques et al. (2010) identified SOC predictions made by ensemble regression trees as more accurate than those derived from PLSR in an investigation in Florida. This suggests that depending on the geographic soil region, one method may outperform several others to make SOC or TC predictions from VNIR spectra.

21.3.2 Factors that Impact the Transferability and Scalability of Prediction Models

Overall, PLSR models performed better to transfer and scale than SVM models (Tables 21.5, 21.6, 21.7, and 21.8). This implies that linear relationships between VNIR spectra and soil TC (quantified by PLSR) were more pronounced than nonlinear, complex relationships (quantified by SVM). Reasons that constrain the transferability and scaling of soil prediction models may be explained by differences in the (i) spectral data domain space, (ii) soil attribute domain space, (iii) methods that determine the internal model structure of VNIR-TC relationships, and (iv) environmental domain space of attributes that control soil carbon dynamics (i.e., soil-forming factors).

21.3.2.1 Spectral Data Domain Space

The transferability and scaling of models may be also dependent on the spectral data domain. The VNIR models to predict TC selected variables in the spectral regions of the absorption features of C–H, N–H, and O–H groups, similar to the VNIR models presented by Vasques et al. (2008, 2009, 2010). These spectral

Table 21.5 The transferability of partial least squares regression (PLSR) models developed in one of the five study fields to predict the soil logTC (log %) of the other four fields

Models	Validation datasets (n = 112)	R^2	Bias (log %)	RMSE (log %)	RPD	RPIQ
Model 1	Field 2	0.53	−0.15	0.19	0.83	1.27
	Field 3	0.51	−0.16	0.21	0.66	0.68
	Field 4	0.17	−0.34	0.36	0.32	0.33
	Field 5	0.11	0.01	0.17	0.64	0.95
Model 2	Field 1	0.15	0.01	0.11	0.99	1.36
	Field 3	0.39	−0.10	0.18	0.74	0.77
	Field 4	0.15	−0.01	0.17	0.67	0.70
	Field 5	0.17	−0.23	0.27	0.40	0.59
Model 3	Field 1	0.12	0.28	0.31	0.37	0.51
	Field 2	0.09	−0.46	0.58	0.28	0.42
	Field 4	0.02	−0.21	0.34	0.34	0.35
	Field 5	0.02	0.01	0.20	0.54	0.80
Model 4	Field 1	0.34	0.34	0.35	0.32	0.44
	Field 2	0.29	0.05	0.15	1.09	1.67
	Field 3	0.32	0.19	0.23	0.59	0.61
	Field 5	0.34	0.19	0.21	0.51	0.75
Model 5	Field 1	0.24	0.37	0.39	0.29	0.41
	Field 2	0.28	0.05	0.16	0.98	1.49
	Field 3	0.25	−0.23	0.28	0.48	0.50
	Field 4	0.22	0.07	0.14	0.82	0.85

R^2 = coefficient of determination; RMSE = root-mean-squared deviations; RPD = residual prediction deviation; RPIQ = ratio of prediction error to inter-quartile range

signatures are produced by the overtones and combinations of absorption molecular vibrations (e.g., C–H, O–H, H_2O, and CO_{3^-}) in mid-infrared regions (Brown et al. 2005). The features associated with TC can be masked or distorted by Fe-oxides and secondary clays which are commonly found in soils (Clark 1999). This alludes to a critical issue of VNIR-modeling that other soil properties, such as texture, nutrient content, and minerals, may mask or interfere with the prediction of a given property of interest (e.g., soil TC) and thus impact the transferability of models. In this study, the soil texture differed only slightly among the five fields with sand content ranging between 90.8 and 98.6 % and clay content between 1.2 and 5.2 %. Hence, the effect of soil texture imposed on TC-spectral signatures was likely minor. However, the soil suborders differed among sites with Entisols (Psamments), Ultisols (Aquults, Udults), Inceptisols (Udepts), and Spodosols (Aquods) (Table 21.1), suggesting that the mineralogy, sesquioxides, and other chemical and physical soil properties differed substantially among sites.

Table 21.6 The transferability of support vector machine (SVM) models predicting soil logTC (log %) developed in one of the five study fields to predict the soil logTC (log %) of the other four fields

Model	Test datasets (n = 112)	R^2	Bias (log %)	RMSE (log %)	RPD	RPIQ
Model 1	Field 2	0.13	−0.47	0.49	0.32	0.49
	Field 3	0.12	−0.06	0.15	0.93	0.96
	Field 4	<0.01	−0.28	0.30	0.38	0.39
	Field 5	0.31	−0.48	0.49	0.22	0.33
Model 2	Field 1	0.06	0.39	0.40	0.28	0.39
	Field 3	0.17	0.37	0.39	0.35	0.36
	Field 4	<0.01	0.14	0.18	0.62	0.65
	Field 5	0.21	−0.06	0.12	0.88	1.30
Model 3	Field 1	0.33	0.09	0.14	0.81	1.12
	Field 2	0.01	−0.38	0.41	0.39	0.60
	Field 4	0.02	−0.19	0.22	0.52	0.54
	Field 5	0.27	−0.39	0.41	0.27	0.40
Model 4	Field 1	<0.01	0.28	0.30	0.38	0.52
	Field 2	<0.01	−0.18	0.24	0.67	1.02
	Field 3	0.06	0.23	0.27	0.51	0.53
	Field 5	0.18	−0.20	0.22	0.49	0.72
Model 5	Field 1	0.04	0.46	0.47	0.24	0.33
	Field 2	<0.01	0.00	0.16	1.00	1.53
	Field 3	0.05	0.41	0.43	0.32	0.33
	Field 4	<0.00	0.19	0.22	0.51	0.53

R^2 = coefficient of determination; RMSE = root-mean-squared deviations; RPD = residual prediction deviation; RPIQ = ratio of prediction error to inter-quartile range

21.3.2.2 Soil Attribute Domain Space

The soil attribute space, i.e., the upper and lower bounds and dispersion of soil TC used to build spectral-based prediction models (Table 21.2), may explain some of the transferability and scalability behavior of models. Typically, the soil attribute domain space expands as the geographic size of the modeled region increases (Grunwald et al. 2011). The range of soil TC values of CAL, VAL, and the SUB-W sets matched reasonably well the min. of 0.31 % and max. of 3.55 % of the Whole dataset. However, the differences in soil TC among field sites were profound. Ideally, the boundary conditions of attributes used for model development of a transfer function (or calibration spectral model) matches the boundary conditions of a transfer set. Brown et al. (2005) demonstrated the limitations of spectral-based model transfer to predict soil carbon in fields in Montana, USA, where the SOC values differed widely among field sites (min. of 1.93 g kg^{-1} to max. of 15.82 g kg^{-1}).

In this study, PLSR Models 1, 3, and 4 that resembled the TC range of SUB-W most closely with TC min. of 0.32 % and TC max. of 2.85 % did not show

Table 21.7 The downscaling performance of the partial least squares regression (PLSR) and support vector machine (SVM) models predicting soil logTC (log %) developed at regional scale (SUB-W) predicting samples at field scales

Model	Validation datasets (n = 112)	R^2	Bias (log %)	RMSE (log %)	RPD	RPIQ
PLSR models						
Model SUB-W (n = 112)	Field 1	0.42	<0.01	0.11	1.07	1.47
	Field 2	0.47	−0.02	0.13	1.27	1.93
	Field 3	0.32	0.07	0.16	0.87	0.90
	Field 4	0.51	−0.04	0.10	1.10	1.14
	Field 5	0.20	−0.03	0.16	0.68	1.00
SVM models						
Model SUB-W (n = 112)	Field 1	0.35	0.08	0.12	0.92	1.26
	Field 2	0.55	−0.08	0.13	1.19	1.81
	Field 3	0.26	0.08	0.14	0.95	0.99
	Field 4	0.65	0.01	0.07	1.63	1.69
	Field 5	0.51	−0.03	0.08	1.32	1.94

R^2 = coefficient of determination; RMSE = root-mean-squared deviations; RPD = residual prediction deviation; RPIQ = ratio of prediction error to inter-quartile range; SUB-W = the 112 observations randomly chosen from the five fields (Fig. 21.1)

persistent responses in terms of transferability (Table 21.5). For example, Model 3 (developed in Pineland and Psamments) failed to transfer well to Field 4, whereas the opposite was found for the transfer behavior of Model 4 (developed in Improved Pasture and Udults) to Field 3. These findings were confounded in down- and upscaling mode (Tables 21.7 and 21.8).

Besides the upper and lower bounds of attributes that matter for successful model transfer and scaling, it is also the internal variability (variance) of soil attributes that potentially impacts behavior. McBratney (1998) and Grunwald et al. (2011) asserted that an increase in the variance of soil attributes can impact the model building process, transferability, and scalability of soil properties. In this study, the coefficient of variation (CV) ranged from 0.26 % (Field 5) to 0.42 % (Field 3) which was lower than in the pooled sets (0.53 % in SUB-W and 0.55 % in whole, respectively). Effects of variability in TC on transfer and scalability of TC models are evident (compare CVs in Table 21.2 and results in Tables 21.5, 21.6, 21.7, and 21.8).

21.3.2.3 Model Structure

Regression methods use different strategies to relate predictors (here: spectral data) and a response variable (here: soil TC). The underlying strategies for predictor selection are different for PLSR and SVM impacting transfer and scale responses.

Table 21.8 The upscaling performance of the partial least squares regression (PLSR) and support vector machine (SVM) models predicting soil logTC (log %) developed at field scale predicting samples at regional scale (SUB-W)

Models	Validation dataset	R^2	Bias (log %)	RMSE (log %)	RPD	RPIQ
PLSR models						
Model 1	SUB-W (n = 112)	0.53	−0.12	0.22	1.09	1.97
Model 2		0.64	−0.03	0.15	1.58	2.87
Model 3		<0.01	−0.17	0.50	0.48	0.86
Model 4		0.57	0.18	0.23	1.02	1.84
Model 5		0.36	0.06	0.23	1.02	1.86
SVM models						
Model 1	SUB-W (n = 112)	0.08	−0.27	0.35	0.67	1.22
Model 2		0.19	0.15	0.27	0.90	1.63
Model 3		0.04	−0.18	0.29	0.81	1.48
Model 4		0.11	0.03	0.23	1.05	1.91
Model 5		0.15	0.21	0.31	0.77	1.40

R^2 = coefficient of determination; RMSE = root-mean-squared deviations; RPD = residual prediction deviation; RPIQ = ratio of prediction error to inter-quartile range; SUB-W = the 112 observations randomly chosen from the five fields (Fig. 21.1)

If the internal model structure that describes the relationship between spectral predictors and soil TC is not stable when it is scaled, it suggests scale-variant behavior. The PLSR and SVM models predicting logTC showed significant differences in the selection of spectral predictors in Models 1 to 5 and the SUB-W Model (results not shown). Thissen et al. (2004) has found major differences in the selection of spectral predictors that are inherent to the modeling process of PLSR and SVM, specifically in cases where the physico-chemical composition of the soil samples differed. In this study, PLSR was more robust than SVM to transfer models among sites. The PLSR models mainly focused on three regions to identify spectral predictors: ~350, ~1860, and ~2200 nm, which represented the reflection region of organic matter (Galvao and Vitorello 1998); O–H, water, C–H, C–N, C–O, N–H (Vasques et al. 2008); and calcium carbonate (2206 and 2341 nm) (Lagacherie et al. 2008), and various C–O (Brown et al. 2005). On the other hand, the top 50 important spectral wavelengths of the SVM models were found around ~670, ~1400, ~1800, and ~2200 nm. Although SVM is advantageous to model complex, high-dimensional spectral datasets because it can model nonlinear structures it performed poorly to transfer and upscale models (Tables 21.6 and 21.8). This can be explained by the high susceptibility of SVM to overfitting (Hernández et al. 2009). The substantially larger amount of spectral values selected as important in the SVM model compared to the PLSR model suggests overfitting.

21.3.2.4 Environmental Domain Space of Attributes

Soil carbon gains/losses have been linked to various environmental factors such as climate (Hook and Burke 2000), land use/land cover (John et al. 2005), soil moisture/hydrology (Vasques et al. 2012a, b), and topography (Yimer et al. 2006). Mallavan et al. (2010) asserted that the more similar regions (fields) are in terms of soil–environmental properties the more likely it is to successfully transfer a soil prediction model. The soil–environmental factors of fields differed widely in terms of topography, climate, parent material, organism/biota, and soils (Table 21.1). The homology among soil–environmental conditions explained a substantial amount of the ability to transfer TC models to other field sites and scales in this study (Fig. 21.2 and Table 21.9). Minasny et al. (2009) found that the transfer of mid-infrared spectral SOC prediction models among three different regions in Australia did not perform well due to differences in parent material and climate in which soils have formed in Queensland, New South Wales, and Victoria. Although the R^2 of transferred models were still moderate, all models showed significant bias. Studies that test not only for similarity in soil TC among sites, but also consider the similarity in environmental factors that form soil carbon are still rare in the soil science literature.

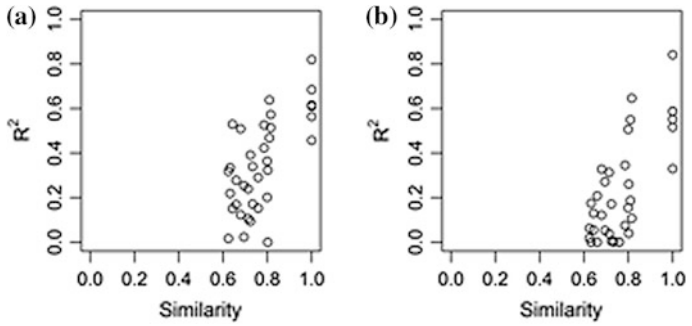

Fig. 21.2 The coefficient of determination (R^2) of each model transferred to other fields and scale versus the Gower similarity coefficient between the model development field/scale and the model application field/scale: **a** partial least squares regression (PLSR); **b** support vector machine (SVM)

Table 21.9 Gower similarity coefficients of soil–environmental factors among fields and across scales (SUB-W)

	Field 1	Field 2	Field 3	Field 4	Field 5	SUB-W
Field 1	1.00	0.64	0.68	0.73	0.71	0.78
Field 2	–	1.00	0.72	0.76	0.66	0.81
Field 3	–	–	1.00	0.62	0.69	0.80
Field 4	–	–	–	1.00	0.63	0.81
Field 5	–	–	–	–	1.00	0.80
SUB-W	–	–	–	–	–	1.00

SUB-W = the 112 observations randomly chosen from the five fields (Fig. 21.1)

21.4 Conclusions

This study showed that, although the spectral models to predict soil TC with different methods (PLSR and SVM) were successful in calibration and validation modes at five different fields nested within a large sand-dominated region in the USA, the transferability and up- and downscaling of models were limited by several factors. All of them interacted with each other impacting the transferability of models among field sites, upscaling, and downscaling behavior of spectral soil prediction models. These findings have implications for the development of 'universal' spectral-based soil models aiming to predict soil properties for a diverse set of different soils formed in different environmental conditions covering a wide range of geographic settings, at its extreme the whole globe. Those 'universal' spectral libraries are based on the premise that soil predictions (e.g., soil TC) can be made anyplace because they are built using soil spectral datasets that characterize exhaustively the attribute feature space. This assertion is limited by the fact that a large number of interacting factors of soils, spectra, and environmental properties are needed to represent the exhaustive sample population which has not materialized yet. Furthermore, the stationarity in mean and variance in local (field) calibrations of spectral soil prediction models are usually easier to meet though can have severe effects on scale-variant behavior of models at escalating spatial scales. The confounding trends in TC up- and downscaling behavior found in this study suggest that scale matters indicating the need for further soil scaling studies. Given the many factors that can impinge on empirically derived soil spectral prediction models, as demonstrated by this study, more focus on the applicability and scaling of them is needed. This study juxtaposed local and regional predictions, transferability, and scalability of soil TC models derived from VNIR spectra within a subtropical region in the southeastern USA. The constraints of soil spectral models identified in this research may also be found in other regions and spectral libraries that intent to have universal applicability.

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