

Developing Soil Cation Exchange Capacity Pedotransfer Functions using Regression and Neural Networks and the Effect of Soil Partitioning on the Accuracy and Precision of Estimation

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ABSTRACT

Soil fertility measures such as cation exchange capacity (CEC) may be used in upgrading soil maps and improving their quality. Direct measurement of CEC is costly and laborious. Therefore, indirect estimation of CEC via pedotransfer functions may be appropriate and effective. Several delineations of two consociation map units consisting of two soil families (Shahrak series and Chaharmahal series), located in Shahrekord plain, Iran were identified. Soil samples were taken from two depths of 0-20 and 30-50 cm and were analyzed in lab for several physico-chemical properties. Clay and organic matter percentages as well as moisture content at -1500 kpa best correlated with CEC. Pedotransfer functions were successfully developed using regression and neural networks. Soil partitioning increased the accuracy and precision of functions. Compared to regression, neural network technique resulted in pedotransfer functions with higher R^2 and lower RMSE.

Keywords: Cation Exchange Capacity (CEC), Pedotransfer, Regression, Neural network, Soil partitioning

INTRODUCTION

There is an increasing demand for reliable large-scale soil data to meet the requirement of models for planning of land-use systems, characterization of soil pollution, and prediction of land degradation (Mc Bratney et al., 2002). Cation Exchange Capacity (CEC) is among the most important soil properties that is required in soil databases (Manrique et al., 1991), and is used as an input in soil and environmental models (Keller et al., 2001). Cation Exchange Capacity is the total of the exchangeable cations that a soil can hold at a specified pH. Soil components known to CEC are clay and organic matter, and to a lesser extent, silt (Martel et al., 1978; Manrique et al., 1991).

Soil fertility measures such as CEC may be used for upgrading soil maps and improving their quality. Simulation models such as the Erosion-Productivity impact calculator (Williams et al., 1989) require large amounts of soil physical and chemical data and CEC is one key property used in this issue.

Although CEC can be measured directly, its measurement is difficult, time consuming and expensive especially in the semiarid region of Iran because of the large amounts of calcium carbonate. Pedotransfer Functions (PTF_s) provide an alternative by estimating CEC from more readily available soil data. The term pedotransfer function was coined by Bouma (1989) as translating data we have in to what we need. In recent years, several researchers tried to estimate CEC from basic physical and

chemical soil properties (Breeusma et al., 1986; Manrique et al., 1991; Bell and Keulen, 1995; McBratney et al., 2002). In most of these models, CEC is assumed to be a linear function of soil organic matter and clay content (Breeusma et al., 1986; McBratney et al., 2002). Results show that greater than 50% of the variation in CEC could be explained by the variation in clay and organic C content for several New Jersey soils (Drake and Motto, 1982), for some Philippine soils (Sahrawat, 1983), and for four soils in Mexico (Bell and Keulen, 1995). Only a small improvement was obtained by adding pH to the model for four Mexican soils (Bell and Keulen, 1995). In B horizons of a toposequence, the amount of fine clay was shown to explain a larger percent of the variation in CEC than the total clay content (Wilding and Rutledge, 1996).

Multiple Linear Regression (MLR) analysis is generally used to find the relevant coefficients in the model equations. Often, however, models developed for one region may not give adequate estimates for a different region (Wagner et al., 2001). Because the most essential input variables can be found automatically using stepwise regression, initially, linear and polynomial regressions were applied (Pachepsky and Rawls, 1999).

A recent approach to model PTF_s is the use of artificial neural networks (ANN_s) (Schaap et al., 1998). Artificial neural networks have been successfully employed to predict soil hydrological properties (Pachepsky and Rawls, 1999; Minasny and McBratney, 2002). A type of ANN known as multilayer perceptron (MLP), which uses a back-propagation training algorithm, is usually used for generating PTF_s (Schaap et al., 1998; Minasny and McBratney, 2002; Amini et al., 2005). An advantage of using ANN_s is that no specific type of function needs to be assumed a priori to model the relationship between inputs and outputs. The optimum relation that links input data to output data is obtained through a training procedure (Schaap et al., 1998). Because of their greater feasibility, ANN models are generally expected to be superior to MLR models (Schaap et al., 1998; Minasny et al., 1999). The drawback of ANN_s is that they do not provide an explicit procedure to select the most essential PTF input variables (Pachepsky et al., 1996).

The PTF accuracy is assessed from the correspondence between measured and estimated data for the data set from which a PTF has been characterized by various quantitative measures, such as the mean error, the standard deviation of the mean error, the mean squared error, determination coefficient R^2 , etc. (Kern, 1995; Leenhardt, 1995). Results show that when soils are grouped by similarities in origin or properties, accuracy of predictive models has been shown to improve (Pachepsky and Rawls, 1999). Examples of soil grouping include lithomorphoc classes (Franzmeier, 1991), hydraulic-functional horizons (Wosten et al., 1985), genetic classification (Leenhardt, 1995), texture classes (Clapp and Hornberger, 1978) and numerical soil classification (Williams et al., 1983). Drake and Motto (1982) grouped soils by taxonomic order or province. Similarly, Asadu and Akamigbo (1990) predicted CEC from organic matter and clay content by grouping the soil based on taxonomic order

(Inceptisols, Alfisols, Ultisols, and Oxisols). The U.S. Soil Taxonomy systems (Soil Survey Staff, 1999) also classifies soils by mineralogical composition at the family level which may be useful in soil partitioning to improve both accuracy and reliability of predictive models (Pachepsky and Rawls, 1999). The objectives of this study were (1) developing of PTFs for CEC using methods of regression and neural networks, (2) studying the possibility of upgrading the soil maps by determining the CEC for two dominant soil families in soil mapping units in Chaharmahal-va-Bakhtiari province and (3) assessing the effect of soil partitioning into families and different layers on the quality of the models.

MATERIALS and METHODS

The study area consists of several irrigated lands in Chaharmahal-Va-Bakhtiari province, Central Iran (Fig. 1). The soil moisture and temperature regimes of the area are xeric and mesic, respectively. One hundred and twenty samples were collected from several delineations of two consociation map units consisting of two soil families (Shahrak series and Chaharmahal series) located in Shahrekord plain, Central Iran. Dominant soils at two consociation map units are classified as follow at family levels:

- 1) *Fine, Mixed, active, Mesic Typic Calcixerepts*
- 2) *Fine, Carbonatic, Mesic Typic Calcixerepts*

The classification of these soils are similar up to subgroup level but their family was different because of difference in mineralogy class.

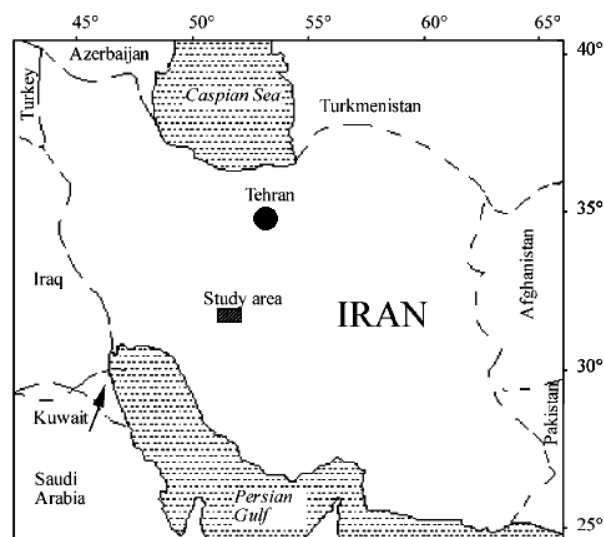


Fig. 1. Location of the study area in Central Iran

Soil samples were taken from two depths of 0-20 and 30-50 cm and were analyzed in lab for several physico-chemical properties including soil particle size distribution, organic matter, moisture content at wilting point at -1500 KPa, pH, calcium carbonate equivalent and cation exchange capacity. Statistical analysis and multiple regressions were performed by STATISTICA 6.0 software and neural network models were developed by JMP 5.0 software. Prediction models were developed at first for

all data without partitioning and then for each family and also surface and subsurface layers. The best linear regression models suggested by researchers for each level (each family, each layer and all samples) were considered for model developing.

The MLP algorithm developed in this study is a feed forward back propagation network (FFBP) model. This network consists of layers of interconnected non linear processing elements called neurons. The architecture of the MLP model is such that the numbers of input and output neurons are usually matched to the numbers of input and output elements. The transfer function was selected a sigmoidal function that is selected such that it accommodates the nonlinearity of the specific input–output relationship. Profiler diagram possibility was used to select suitable number of node in the hidden layer and avoid under fitting and over fitting.

The performance of the models was evaluated using the root mean square error (RMSE) and the correlation coefficient (R^2) between predicted and measured values. Relative improvement (RI) index was used to compare the performance of two models developed from regression and neural networks.

RESULTS and DISCUSSION

Descriptive Analysis

The summary statistics of the soil properties for two families are given in Tables 1 and 2.

Table 1. Summary statistics of soil properties for family one

property	Mean			Max	Min	CV%	Mean of two layers	
	Surface Layer	Depth Layer	Family				Difference *	Significant Level
%Sand	17.8	16.4	17.1	35.3	5.7	39.7	1.4	ns
%Silt	42.7	39.7	41.2	65.4	27.3	22.8	3	ns
%Clay	33.7	45.3	39.5	63.7	24.6	21.7	-11.6	99%
%OM	1.8	1.1	1.4	2.9	0.32	34.7	0.73	99%
%PWP	19.2	19.3	19.2	27.6	12.4	16.6	-0.1	ns
%CaCO ₃	22.1	25	23.4	39.0	12.5	28.2	-2.9	ns
pH	7.8	8	7.9	8.4	7.2	2.5	-0.1	ns
CEC (cmol _c kg ⁻¹ soil)	36.5	37	36.7	69.2	14.7	39.8	-0.5	ns

* The negative difference means that quantity of properties in depth layer is greater than surface layer

Table 2. Summary statistics of soil properties for family two

property	Mean		Max	Min	CV%	Mean of two layers		
	Surface Layer	Depth Layer				Family	Family	Difference *
%Sand	25.4	24.4	24.9	42.6	11.5	22.6	0.1	ns
%Silt	41.4	36.9	39.1	53.6	22.0	15.7	4.5	ns
%Clay	32.8	40.5	36.7	49.7	24.6	11.3	-7.7	99%
%OM	1.6	0.94	1.27	2.4	0.63	18	0.7	99%
%PWP	20.0	19.4	19.7	26.5	12.4	13.6	0.6	ns
%CaCO ₃	23.0	31.2	27.1	45.0	14.0	27.3	-8.3	ns
pH	7.6	7.7	7.7	8.0	7.1	3.6	-0.1	ns
CEC (<i>cmol_c kg⁻¹ soil</i>)	31.5	30.56	31.0	71.4	9.7	54.4	0.9	ns

* The negative difference means that quantity of properties in depth layer is greater than surface layer

The organic matter content of the soils in the region is usually low, ranging from 0.32 to 2.9% and 0.63 to 2.4% for families one and two, respectively with an average of 1%. The coefficient of variation (CV) of CEC showed more variability than those of the soil particle size distribution, OM, pH and PWP in two families. A mean difference (L=0.99%) was observed for OM and clay contents between layers in two families (Tables 1 and 2). Significant difference between clay content in two layers is probably due to more clay in depth layers of each family because of transmission clays from epipedon toward endopedon (Arnaud and Septon, 1972). These results were in general agreement with those of Nourbakhsh et al. (2002) who obtained significant difference for OM and clay contents between two horizons.

Correlation of Soil Properties

The linear correlation coefficients between CEC and independent variables are given in Table 3.

Table 3. Simple linear correlation coefficients (r) between CEC and independent variables

Partitioning Level	OM	PWP	Clay	Sand	Silt	CaCO ₃	pH
	%						
All Samples (No Partitioning)	0.53*	0.73*	0.51*	-0.30*	0.16	-0.15	0.10
Family one	0.58*	0.78*	0.51*	-0.20	0.11	-0.17	0.07
Surface layer of family one	0.89*	0.77*	0.66*	-0.23	0.32	-0.29	0.03
Depth layer of family one	0.70*	0.80*	0.73*	-0.16	0.17	-0.01	0.11
Family two	0.50*	0.75*	0.53*	-0.29	0.19	-0.07	0.02
Surface layer of family two	0.86*	0.76*	0.58*	-0.21	0.04	-0.03	0.05
Depth layer of family two	0.82*	0.76*	0.81*	-0.35	0.31	-0.15	0.00

*The relation is significant at the 0.05 level.

This table shows OM, clay and PWP has higher correlations with CEC (L=95%) among the measured properties. As expected, the correlations between the CEC and sand content were negative. Positive correlation between CEC, soil OM and clay content is related to existence of negative charges on these properties (Manrique et al., 1991; Bell and Keulen., 1995 and Noorbakhsh et al., 2005). Positive significant correlation between CEC and PWP may be explained by the same influence of OM and clay on them. Najafi (2005) also observed high correlation coefficient between CEC and PWP (r=0.90) in his results.

The correlation coefficient between CEC and OM in each family decreased from surface layer to depth layer, whereas the correlation coefficient between CEC and clay in each family increased from surface to depth layer (Table 3). It seems that existence of more OM in surface layer and more clay in depth layer is the main reason for significant correlation coefficients in this layer. These results are similar to the results of several researchers (Wilding and Rutledge, 1966; Noorbakhsh et al., 2005). In general, partitioning each family in to layers caused to increasing significant correlation coefficients for CEC, clay and OM. The partitioning of soils in to family and layer could not effect on correlation coefficient between CEC and PWP (Table 3).

Developing Soil CEC PTFs using Regression

The following models suggested by researchers in literature review were used for calibration of the soils in our study area:

Model 1: $CEC = B_0 + B_1 \%OM$ (Bell and Keulen, 1995; Noorbakhsh et al., 2005)

Model 2: $CEC = B_0 + B_1 \%Clay$ (Bell and Keulen, 1995)

Model 3: $CEC=B_0+B_1 \%Clay + B_2\% OM$ (Martel et al., 1977; Bell and Keulen, 1995; Noorbakhsh et al., 2005)

Model 4: $CEC=B_0+B_1 \%OM+B_2\%PWP$ (Seybold et al., 2005)

The results of calibration and its accuracy are given in Tables 4 to 7.

Table 4. Test results of the regression for model 1.

Number	Partitioning Level	Calibration coefficients		R^2	RMSE
		B_0	B_1		
1	No Partitioning	8.7	18.5	0.28	14.0
2	Surface layers of two families	-28	36.4	0.75	8.8
3	Depth layers of two families	49.7	-16.2	0.52	11.8
4	Family one	14.1	15.75	0.31	12.3
5	Surface layer of family one	-20	31/6	0.79	7.4
6	Depth layer of family one	0.32 ^a	34.12	0.47	10.1
7	Family two	3.6 ^a	21.5	0.25	15.9
8	Surface layer of family two	-48.4	49.8	0.73	9.0
9	Depth layer of family two	-45	80.86	0.67	11.3

^a The coefficients are not significant at the 0.05 level

Without partitioning, models (1) and (2) predicted CEC weakly. Results showed that although soil partitioning in to families didn't improve accuracy of models (1) and (2), partitioning each families in to layers caused to increase R^2 and decrease the RMSE. However, model (1) for upper layer and model (2) for depth layer were more suitable. These results accord well with correlation of CEC with OM and clay in Table 3. It seems that using simultaneous variables of OM and clay percentage caused to make better estimation for CEC (Model 3, Table 6). Accuracy of model 3 without partitioning is also higher than models 1 and 2. Comparison the R^2 and RMSE of model 3 with models 1 and 2 showed an increase of R^2 from 0.28 to 0.67 and a decrease of RMSE from 14 to 9.5.

Table 5. Test results of the regression for model 2.

Number	Partitioning Level	Calibration coefficients		R^2	RMSE
		B_0	B_1		
10	No Partitioning	-10.8 ^a	1.17	0.28	14.3
11	Surface layers of two families	-46	2.2	0.38	13.0
12	Depth layers of two families	-46	1.85	0.54	11.5
13	Family one	2.3a	0.87	0.26	12.7
14	Surface layer of family one	-29.4 ^a	2	0.43	12.2
15	Depth layer of family one	-25.4	1.37	0.54	9.4
16	Family two	-28	1.6	0.28	15.5
17	Surface layer of family two	-56.6	2.7	0.34	14.1
18	Depth layer of family two	-91.25	3	0.65	11.6

^a The coefficients are not significant at the 0.05 level

Table 6. Test results of the regression for model 3.

Number	Partitioning Level	Calibration coefficients			R^2	RMSE
		B_0	B_1	B_2		
19	No Partitioning	-51.2	22/8	1.4	0/67	9/5
20	Surface layers of two families	-43	31/7	0.68	0/75	8/4
21	Depth layers of two families	-46.5	29/6	1.17	0/65	10/0
22	Family one	-35.1	19/5	1.11	0.72	7.9
23	Surface layer of family one	-30.97	27/8	0.51 ^a	0.81	7.2
24	Depth layer of family one	-30	20/4	0.97	0.66	8.3
25	Family two	-90	30.65	2.24	0.74	9.4
26	Surface layer of family two	-74.9	43.5	1/1	0.78	8.3
27	Depth layer of family two	-85.2	49	1.7	0.78	9.3

^a The coefficients are not significant at the 0.05 level

Soil partitioning in to family and family in to surface and subsurface layers could improve the quality of model (3) especially in surface layers (Functions no. 23 and 26). An unexpected value for function no. 24 is probably related to existence of different clay minerals. As texture and organic material data are more available and their measurement is more convenient than CEC, the use of the model (3) seems more practical and useful.

When the PWP measurement is possible or the data related to the PWP and the percentage of the OM is accessible, the model (4) may be used (Table 7). The RMSE values in our research are in agreement with Noorbakhsh et al. (2005). Bell and Keulen (1995) reported less RMSE (1.5) and more R^2 (0.85) rather than the results of the present research. Seybold et al. (2005) found the RMSE average of 0.3 and the average of 0.7 for R^2 using two attributes of O.M and clay and exponential models.

Table 7. Test results of the regression for model 4.

Number	Partitioning Level	Calibration coefficients			R^2	RMSE
		B_0	B_1	B_2		
28	No Partitioning	-42.4	15.4	3.3	0.58	10.8
29	Surface layers of two families	-42.6	49	1.6	0.77	8.0
30	Depth layers of two families	-42.2	29.14	2.4	0.66	10.0
31	Family one	-31.5	2.3	3	0.65	8.8
32	Surface layer of family one	-33.5	43	1.28	0.81	7.0
33	Depth layer of family one	-26	2	2.5	0.70	7.8
34	Family two	-57.7	13.2	4	0.60	11.8
35	Surface layer of family two	-66.5	64.5	1.88	0.78	8.3
36	Depth layer of family two	-61.4	97	2	0.73	10.4

Developing Soil CEC PTFs with Neural network

We used same independent variables discussed in regression models as input data and CEC was supposed as only output variable for developing neural networks models. So, the models 1 to 4 were also used for neural network.

Table 8 indicates that the model 3 usually is the best for estimation of CEC in comparison with models 1 or 2 (data not shown). Therefore, O.M and clay contents were suitable inputs for developing soil CEC pedotransfer functions in both neural network and regression methods, Manrique et al. (1991) also concluded that contributions of clay and OM to the prediction of CEC increased significantly when soils were grouped by order. Partitioning soils in to layers especially in each family caused to improve quality of model 4 like regression method (Table 9).

Table 8. Test results of the neural network for model 3.

Number	Partitioning Level	R^2	$RMSE$
55	No Partitioning	0.73	0.38
56	Surface layers of two families	0.85	0.38
57	Depth layers of two families	0.75	0.50
58	Family one	0.74	0.51
59	Surface layer of family one	0.90	0.31
60	Depth layer of family one	0.67	0.58
61	Family two	0.77	0.46
62	Surface layer of family two	0.83	0.41
63	Depth layer of family two	0.88	0.34

Table 9. Test results of the neural network for model 4.

Number	Partitioning Level	R^2	$RMSE$
64	No Partitioning	0.63	0.60
65	Surface layers of two families	0.85	0.38
66	Depth layers of two families	0.72	0.53
67	Family one	0.68	0.56
68	Surface layer of family one	0.90	0.30
69	Depth layer of family one	0.73	0.52
70	Family two	0.65	0.57
71	Surface layer of family two	0.82	0.42
72	Depth layer of family two	0.83	0.41

Comparison of regression PTFs with neural networks

Relative Improvement shows R^2 and $RMSE$ values of the models in all levels of separation heavily decrease. This means that the neural network for CEC estimates has more accuracy.

Amini et al. (2005) also indicate that using the neural network model with FFBP algorithm toward regression method estimates CEC with high accuracy. Our results with one node showed greater R^2 and less $RMSE$ in comparison with their results. It seems that the main reason for higher accuracy is soil partitioning and more homogeneity of soils.

CONCLUSION

Soil partitioning increased the accuracy and precision of functions. The main reason for increasing the accuracy of models is increasing the homogeneity and uniformity of soil properties.

In both regression and neural network methods, concurrent input of clay and OM caused higher accuracy for estimation of CEC. Compared to regression, neural network technique resulted in pedotransfer functions with higher R^2 and lower RMSE. Upgrading soil maps may be done by developing models of estimation for time consuming and costly variables.

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