

## Comparison of multiple linear regressions and artificial intelligence-based modeling techniques for prediction the soil cation exchange capacity of Aridisols and Entisols in a semi-arid region

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### Abstract

The cation exchange capacity (CEC) of the soil is a basic chemical property, as it has been approved that the spatial distribution of CEC is important for decisions concerning pollution prevention and crop management. Since laboratory procedures for estimating CEC are cumbersome and time-consuming, it is essential to develop an indirect approach such as pedo-transfer functions (PTFs) for prediction this parameter from more readily available soil data. The aim of this study was to compare multiple linear regressions (MLR), adaptive neuro-fuzzy inference system (ANFIS) and artificial neural network (ANN) including multi-layer perceptron (MLP) and radial basis function (RBF) models to develop PTFs for predicting CEC of Aridisols and Entisols in Khuzestan province, southwest Iran. Five soil parameters including bulk density, calcium carbonate, organic carbon, clay and silt were considered as input variables for proposed models. The prediction capability of the models was evaluated by means of comparison with observed data through various descriptive statistical indicators including mean square error (MSE) and determination coefficient ( $R^2$ ) values. Results revealed that the MLP model ( $R^2=0.83$ ,  $MSE=0.008$ ) had the most reliable prediction when compared with the other models. Also results indicated that the ANFIS model ( $R^2=0.50$ ,  $MSE=0.009$ ) had approximately similar accuracy with those of MLR ( $R^2=0.51$ ,  $MSE=1.21$ ), while, their prediction performance was less than RBF ( $R^2=0.74$ ,  $MSE=0.034$ ) model. However, regarding to obtained statistical indicators, ANNs especially MLP model provide new methodology with acceptable accuracy to estimate the CEC of Aridisols and Entisols that diminished the engineering effort, time and funds.

**Keywords:** Adaptive neuro-fuzzy inference system, artificial neural network, cation exchange capacity, multiple linear regressions.

**Abbreviations:** ANFIS= adaptive neuro-fuzzy inference system, ANN= artificial neural network, CEC= cation exchange capacity, MLP= multi-Layer perceptron, PTFs= pedo-transfer functions, RBF= radial basis function.

### Introduction

The cation exchange capacity of a soil is the number of moles of adsorbed cation charge that can be desorbed from unit mass of soil, under given conditions of temperature, pressure, soil solution composition and soil-solution mass ratio (Sposito, 1989). In other words cation exchange capacity or CEC, refers to the quantity of negative charges in soil. The negative charge may be pH dependent (soil organic matter) or permanent (some clay minerals) (Evans, 1989). Cation exchange capacity along with FC and PWP are among the most important soil properties that are required in soil databases (Manrique et al, 1991). It has been approved that soil CEC obviously influences plenty of soil properties as it is vital to predict the potential for pollutant sequestration in the environment (Tang et al., 2009). Since many essential plant nutrients exist in the soil as cations such as potassium ( $K^+$ ), calcium ( $Ca^{2+}$ ), magnesium ( $Mg^{2+}$ ), and ammonium ( $NH_4^+$ ), therefore, the CEC is a very important soil property for nutrient retention and supply. In addition, the exchange cations of organo-mineral particle-size fractions act as bridges between soil and plant (Caravaca et al, 1999). According to Matula (2009) The CEC value contributes to a more sophisticated approach to interpretation for the fertilizer recommendations. The swelling properties of the soils are affected by CEC. In other words, the swelling capacity is

closely related to the CEC. The amount of swelling increases with increasing CEC (Christidis, 1998). In the laboratory procedure, CEC of the soils is measured by using the ammonium acetate ( $NH_4OAc$ ) method through the replacement of sodium ( $Na^+$ ) ions with ammonium ( $NH_4^+$ ) ions that is difficult, time consuming and expensive, especially in the aridisols of Iran because of the large amounts of calcium carbonate (Carpena et al., 1972). So, it is essential to provide an alternative approach to estimate CEC from more easily measurable and readily available soil properties such as particle-size distribution (sand, silt and clay content), organic matter or organic C content and bulk density. In soil science, such relationships are referred to as pedo-transfer functions (PTFs) that were coined by Bouma (1989). According to Wösten et al (1995) PTFs represent predictive functions that translate the data we have (input) into the data we need (output). Although there are conventional statistical techniques for developing PTFs (i.e. regression), in recent years several artificial intelligence-based modeling techniques such as artificial neural networks (ANNs), fuzzy inference systems (FIS) evolutionary computation, etc and their hybrids because of their predictive capabilities and nonlinear characteristics have been much popularity as an alternate statistical tool in the modeling of various complex environmental problems (Yilmaz and

Kaynar, 2011). Several attempts have been conducted in relation to modeling various soil physiochemical parameters by means of different artificial intelligence-based modeling techniques such as those done for modeling of the daily and hourly behavior of runoff (Aqil et al., 2007), estimating the groutability of granular soils (Tekin and Akbas, 2011), to determine the clay dispersibility (Zorluer et al., 2010), prediction of swell potential of clayey soils (Yilmaz and Kaynar, 2011), modeling of Pb(II) adsorption from aqueous solution (Yetilmezsoy and Demirel, 2008), prediction of soil water retention and saturated hydraulic conductivity (Merduin et al., 2006), estimation of soil erosion and nutrient concentrations in runoff (Kim and Gilley, 2008), land suitability evaluation (Keshavarzi et al., 2011) and etc. Some studies also have it been considered capability of soft computing techniques for modeling soil cation exchange capacity such as those conducted by Amini et al (2005), Tang et al (2009) and Keshavarzi et al (2012). The findings of these researchers demonstrated that PTFs developed through artificial intelligence-based modeling techniques were more efficient than the regression ones to predict the CEC. Since few studies focused on developing PTFs by means of ANFIS for prediction CEC, hence, the main objectives of this research were 1) Application of multiple linear regressions (MLR) and artificial intelligence-based modeling techniques to predict soil CEC. Two widely-used artificial intelligence-based modeling techniques were taken in consideration: adaptive neuro-fuzzy inference systems (ANFIS) and artificial neural networks (ANNs) including multi-layer perceptron (MLP) and radial basis function (RBF) and 2) comparison of the proposed artificial intelligence-based models together and multiple linear regressions by means of various descriptive statistical performance indicators such as  $R^2$  and MSE.

## Results and discussion

### Statistical analysis of data

The descriptive statistical characteristics of the used soil physiochemical properties in the development and validation of PTFs using multiple linear regressions (MLR), artificial neural networks (RBF and MLP) and adaptive neuro-fuzzy inference system (ANFIS) models are summarized in Table 1. As indicated from this table, the CEC values of the studied soil samples ranged between 1.3 and 17.6 with an average value of 13.61 Cmolc/kg. It was found that the OC content of the soils is very low, ranging from 0.1-1.61, with an average of %0.47 and therefore, natural soil fertility is also low. This is because all the studied soils were classified as Entisols and Aridisols based on Soil Survey Staff (2010) as above-mentioned. The limited organic matter that is present can be quickly lost when soils are cultivated for agricultural crop production. Contrary to OC content of the soils, the quantities of soil salinity (EC) were very high with an average of 25.19 ds/m, values varied from 1.45 to 213.3 ds/m. On the other hand, clay with an average of 26.68 (8-46.8) percent among the soil particle-size distribution had higher and less quantities than sand and silt, respectively. Table 2 presents the calculated simple linear correlation coefficients ( $r$ ) between CEC and input variables. It was found that there is a positive and highly significant correlation between CEC with OC and clay percentage, as the observed correlation between CEC and clay (0.566<sup>\*\*</sup>) were more than CEC and OC (0.232). It is demonstrated that most of negative charges in the studied soils were identified as permanent charge. The observed correlation between CEC

and silt (0.047) were less than OC and clay variables (Caravaca et al., 1999; Seybold et al., 2005 and Amini et al., 2005). The observed correlation between CEC and sand percentage was found negative and significant (-0.391<sup>\*\*</sup>). This indicates that existing high sand quantities in soil will decrease CEC. Generally, regarding to obtained correlations between CEC and soil physiochemical properties, it can be concluded that soil CEC is mainly determined by the amount of clay and OM. This is due to the participation of these parameters in producing negative charge and cation exchange phenomena that is pointed out in many previous studies (Manrique et al., 1991; Francois et al., 2004). Moreover, significant correlations between CEC and other soil properties, such as sand, silt, pH, bulk density, and EC, have also been observed (Manrique et al. 1991; Horn et al. 2005; Jung et al. 2006; Igwe and Nkemakosi 2007). In order to develop PTFs using proposed models for prediction CEC, data subdivided into two sets: 80% of the data for training or calibrating, while the remaining 20% was used for testing the performance of the model predictions.

### Multiple linear regressions (MLR)

Developing PTFs using MLR model for predicting soil CEC in Khuzestan province was done by means of SPSS 16 software and above-mentioned physiochemical soil properties were used as independent variables. In the regression analysis, normalizing the data distribution is one of the primary assumptions that have to be carried out. Therefore, the normality of the data was evaluated using the Kolmogorov-Smirnov method. Bulk density and clay data had a normal distribution, while,  $\text{CaCO}_3$ , EC, OC, sand and silt data did not conform to normal distribution and were normalized using the logarithmic and natural-based logarithmic transformations. After normalizing data, multiple linear regression function was derived for training data set through backward method. In this method, all data were first inserted as input data and subsequently the data that were significantly less effective on output parameter were eliminated. Three different MLR models were derived among CEC and soil physiochemical properties (Tables 3 and 4). It was found that the developed equations through MLR model among CEC and input variables were not statistically strong enough to establish significant models by traditional statistical models. However, since the accuracy of pedo-transfer function models depend on the number of inputs, while increasing the number of inputs will decrease the accuracy of the estimations (Schaap et al 1998; Amini et al 2005). Therefore, the best regression equation that was derived for training data set was as Eq. 6:

$$\text{CEC} = 20.85 - 3.21 * \text{B.D} + 0.122 * \text{Clay} + 0.936 * \text{LnOC} - 2.689 * \text{LnCaCO}_3 + 1.33 * \text{LnSilt} \quad (6)$$

After determining regression equation, in order to evaluate the accuracy of MLR model, the results of this model were compared with experimental data. In fact, the coefficient of determination ( $R^2$ ) between the measured and predicted values is a good indicator to check the prediction performance of the model (Gokceoglu and Zorlu, 2004). The obtained values of  $R^2$  and MSE using MLR are shown in Table 5. For test dataset, the  $R^2$  and MSE values have been obtained 0.51 and 1.21, respectively. This is in agreement with the results of Yilmaz et al (2011). However, obtained results were against those reported by Sarmadian et al (2009). Their results showed high correlation coefficient ( $r = 0.78$ ) for predicting the soil CEC by means of multiple linear regression. This is due to that as above-mentioned, the more

**Table 1.** Descriptive statistics of the datasets used for training and testing (MLR, ANN and ANFIS).

Variable	Units	Training data				Testing data			
		Min	Max	Mean	S.D	Min	Max	Mean	S.D
EC	ds m <sup>-1</sup>	1.45	213.3	25.19	37.92	4.1	118	21.24	29.17
OC	%	0.1	1.61	0.47	0.27	0.15	1	0.41	0.23
B.D	gr cm <sup>-3</sup>	1.04	1.6	1.41	0.1	1.16	1.75	1.38	0.15
Caco <sub>3</sub>	%	22.5	58	43.46	7.09	42.7	57	49.25	3.58
Sand	%	0.56	75	23.26	14.01	0.2	56	23.44	16.56
Silt	%	10	76	50	11.51	33.4	72.4	51.61	10.09
Clay	%	8	46.8	26.68	9.02	9.4	39	24.94	9.13
CEC	Cmol kg <sup>-1</sup>	1.3	17.6	13.61	2.35	6.4	19	13.38	3

EC: soil salinity, OC: organic carbon, B.D: bulk density, Caco<sub>3</sub>: calcium carbonate, CEC: cation exchange capacity

**Table 2.** Calculated coefficient correlations between used variables.

variable	EC (ds m <sup>-1</sup> )	OC %	Caco <sub>3</sub> %	Sand %	Silt %	Clay %	B.D gr cm <sup>-3</sup>	CEC (Cmol kg <sup>-1</sup> )
EC (ds m <sup>-1</sup> )	1							
OC %	-0.166	1						
Caco <sub>3</sub> %	0.047	-0.232*	1					
Sand %	-0.106	0.017	-0.303**	1				
Silt %	0.214*	-0.117	0.502**	-0.781**	1			
Clay %	-0.097	0.118	-0.138	-0.630**	0.007	1		
B.D gr cm <sup>-3</sup>	0.306**	0.058	-0.208*	-0.162	0.048	0.200*	1	
CEC (Cmol kg <sup>-1</sup> )	0.094	0.232	-0.184	-0.391**	0.047	0.566**	-0.022	1

\*\* . Correlation is significant at the 0.01 level. \* . Correlation is significant at the 0.05 level.

inputs will result in the less accuracy of the estimation (Schaap et al 1998; Amini et al 2005). Input data in Sarmadian et al (2009) study were clay and OC while in the present study, five variables were considered as input data. The scatter plot of the measured against predicted CEC values obtained from the MLR model for the test data set with a poor correlation coefficient is illustrated in Fig. 2.

#### Artificial neural networks (MLP and RBF)

In order to predict the soil CEC indirectly through ANN model, as above-mentioned two different algorithms of ANN including radial basis function (RBF) and multi-layer perceptron (MLP) models were used in this study. The input data were those employed by MLR model. In order to this end, all data set were first normalized between 0 and 1 to achieve effective network training. Luk et al (2000) stated that neural networks trained on normalized data, achieve better performance and faster convergence in general, although the advantages diminish as network and sample size become large. Normalizing the data set was done through the Eq. 7:

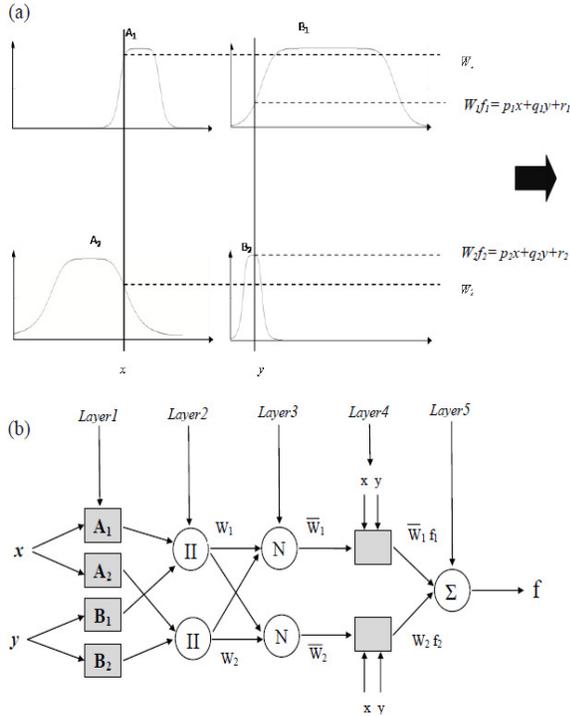
$$x_{norm} = \frac{x - x_{min}}{x_{max} - x_{min}} \quad (7)$$

Where  $x_{norm}$  is the normalized value,  $x$  is the actual value,  $x_{max}$  is the maximum value and  $x_{min}$  is the minimum value.

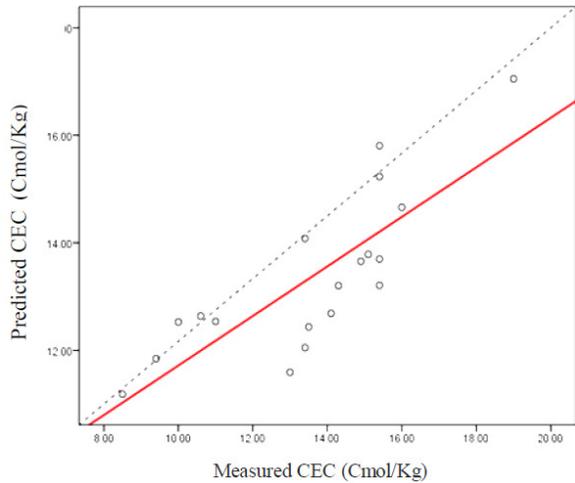
A three-layered feed-forward ANN architecture with an input layer, one hidden layer and an output layer that is schematically represented in Fig. 3 were developed for predicting CEC by means of both ANN models in Khuzestan province. A feed-forward network is a common ANN architecture that requires relatively little memory and is generally fast (Lawrence, 1994). The optimal architecture of each network was determined based on R<sup>2</sup> and MSE values criteria of the trained data set. Table 5 summarizes the results of statistical performance and optimal architecture of ANN networks. For MLP network, the architecture including five neurons in the input layer and one neuron in the output layer

with tangent sigmoid transfer function (tansig) at hidden layer consists of three neurons and a linear transfer function (purelin) at output layer gave the best results. The hidden layer with seventy five neurons was identified as an optimal structure for RBF network, while the number of neurons in input and output layers was the same one for MLP. In order to employ RBF, Gaussian function that is the most widely used in applications, was chosen as a Threshold function for hidden layer. The findings of Chen et al (1991) suggested that the choice of radial basis function used in network does not significantly affect performance of network. The MLP and RBF networks fed with three fourth of the normalized operational data were trained for 350 and 75 epochs, respectively. In the next step, a regression analysis of the network response between ANN outputs and the corresponding targets was performed. As seen from Table 5, the values of R<sup>2</sup> and MSE between ANNs outputs and the corresponding targets indicated that provided predictions using MLP model (R<sup>2</sup>= 0.83, MSE= 0.008) had higher accuracy than RBF ones (R<sup>2</sup>= 0.74, MSE= 0.034). The levels of R<sup>2</sup> and MSE derived by both ANN models for predicting studied soil CEC had higher and less values, respectively, than those derived by multiple linear regressions which were a support for those previous studies conducted by Tamari et al (1996), Minasny and McBratney (2002), Amini et al (2005), Tekin and Akbas (2011) and other researchers. Amini et al (2005) showed that the neural networks PTFs were more efficient than the regression ones to predict the CEC. This is due to that unlike the traditional regression PTFs, ANNs do not require a priori regression model which relates input and output data that in general is difficult because these models are not known (Schaap and Leij, 1998). Also Tamari et al (1996) and Minasny and McBratney (2002) stated that when the number of input parameters is greater than three, ANNs usually perform better than regression techniques, particularly when uncertainties in the quality of the data were small. Additionally, many investigations have indicated that a neural network with one hidden layer is capable of approximating any finite non-linear function with very high

accuracy (Kim and Gilley, 2008; Yimaz and Kaynar, 2011). The scatter plots between experimental and predicted CEC



**Fig 1.** (a) Two input first-order Sugeno fuzzy model with two rules and (b) equivalent ANFIS architecture.



**Fig 2.** Measured CEC (Cmol/Kg) versus Predicted CEC (Cmol/Kg) using MLR.

using MLP and RBF models with acceptable accuracy are indicated in Figs. 4 and 5, respectively.

#### Adaptive neuro-fuzzy inference system (ANFIS)

In this study, ANFIS model was also applied for predicting CEC using the same normalized data that were used for ANN models. In the ANFIS system, each input parameter might be clustered into several class values in layer 1 to build up fuzzy

rules and each fuzzy rule would be constructed using two or more membership functions in layer 2. Several methods have been proposed to classify the input data and to make the rules, among which the most widespread are grid partition and subtractive fuzzy clustering (Aqil et al, 2007; Ertunc and Hosoz, 2008; Yetilmezsoy et al, 2011). In this study, subtractive fuzzy clustering was taken in consideration. The descriptive performance of the ANFIS model for the test data set and the related statistical evolutionary results are given in Fig. 6 and Table 5. The values of 0.5 and 0.009 for  $R^2$  and MSE parameters, respectively, for ANFIS testing stage, show approximately similar prediction accuracy of ANFIS model with the MLR, while its efficiency were less than both ANN models. Generally, results of the comparison of MSE and  $R^2$  indices for predicting CEC showed that prediction performance of the MLP was more than RBF one, while, their predictive performance had higher accuracy than those of ANFIS and MLR models. This is in line with the work done by Yilmaz and Kaynar (2011). Their findings demonstrated that prediction performances of the ANN models (MLP and RBF) had higher accuracy than both multiple regression equations and adaptive neuro-fuzzy inference system for predicting swell potential of clayey soil. Also, results indicated that the ANFIS model for prediction of CEC had approximately similar accuracy when compared with the multiple regression models.

## Materials and methods

### Data collection

This study was carried out in Khuzestan province ( $50^{\circ} 33' N$  to  $47^{\circ} 40' E$ ) located in the south west of Iran. The climate of Khuzestan province varies from arid to humid (Zarasvandi et al, 2011). The determination of numerous chemical and physical properties was carried out on 100 soil samples collected from surface horizons of 100 soil profiles located in Khuzestan Province. Using profile description and laboratory analyses of soil samples, all the studied soils were classified as Entisols and Aridisols on the basis of Soil Survey Staff (2010). The soil properties measured for this study were organic carbon percentage (%OC), calcium carbon content percentage ( $\text{CaCO}_3$ ), soil salinity (EC), cation exchange capacity (CEC), bulk density (B.D) and soil particle-size distribution. The following analytical methods were employed to measure each of parameters for this study: %OC was determined using Walkley-Black method (Nelson and Sommers, 1982), Particle size distribution using pipette method (Gee and Bauder, 1986), CEC using sodium acetate ( $\text{pH} = 8.2$ ) (Thomas, 1982), EC using EC meter (ISWRI, 1998), B.D using clod method (Blake and Hartge, 1986) and %  $\text{CaCO}_3$  by titration method (ISWRI, 1998). The results of determinations were used as input variables to develop the CEC estimation models.

### Multiple regression models

The general purpose of multiple regressions is to learn more about the relationship between several independent or predictor variables and a dependent or criterion variable. Multiple linear regressions (MLR) are the most common method used in development PTFs. The general form of the regression equations is according to Eq. 1:

$$Y = b_0 + b_1 X_1 + \dots + b_7 X_7 + b_8 X_8 + \dots + b_n X_n \quad (1)$$

Where  $Y$  is the dependent variable representing CEC,  $b_0$  is the intercept,  $b_1, \dots, b_n$  are regression coefficients, and  $X_1 - X_n$  are independent variables referring to basic soil properties.

**Table 3.** Coefficients of variables used in MLR models to develop PTFs for prediction CEC.

Model	Independent variables	Coefficient	Std. error	t-Value	Sig. Level
1	Constant	17.012	6.140	2.771	0.007
	B.D	-3.644	1.615	-2.257	0.027
	Clay	0.144	0.025	5.753	0.000
	LogEC	0.289	0.337	0.856	0.395
	LnOC	0.822	0.322	2.553	0.013
	LnSand	0.572	0.428	1.336	0.186
	LnCaCO <sub>3</sub>	-2.931	1.384	-2.117	0.038
	LnSilt	2.016	0.952	2.118	0.038
2	Constant	16.441	6.093	2.698	0.009
	B.D	-3.424	1.591	-2.152	0.035
	Clay	0.144	0.025	5.756	0.000
	LnOC	0.770	0.316	2.439	0.017
	LnSand	0.565	0.427	1.323	0.190
	LnCaCO <sub>3</sub>	-2.931	1.382	-2.121	0.037
	LnSilt	2.153	0.936	2.299	0.024
3	Constant	20.852	5.125	4.069	0.000
	B.D	-3.215	1.591	-2.021	0.047
	Clay	0.122	0.019	6.515	0.000
	LnOC	0.936	0.291	3.217	0.002
	LnCaCO <sub>3</sub>	-2.689	1.377	-1.953	0.055
	LnSilt	1.330	0.703	1.891	0.063

**Table 4.** Performance indices (R<sup>2</sup> and MSE) for different regression models.

Model	Predictors	R <sup>2</sup>	MSE
1	Constant, Ln Silt, Clay, Ln OC, B.D, Log EC, Ln Caco3, Ln Sand	0.57	1.14
2	Constant, Ln Silt, Clay, Ln OC, B.D, Ln Caco3, Ln Sand	0.57	1.13
3	Constant, Ln Silt, Clay, Ln OC, B.D, Ln Caco3	0.56	1.15

**Table 5.** Performance indices (R<sup>2</sup> and MSE) for different models.

Model	Architecture	Threshold function	Training		Testing	
			R <sup>2</sup>	MSE	R <sup>2</sup>	MSE
MLR			0.56	1.15	0.51	1.21
MLP	5-3-1	Tansig-Purelin	0.92	0.002	0.83	0.008
RBF	5-75-1	Gaussian	0.77	0.007	0.74	0.034
ANFIS			0.55	0.009	0.50	0.009

### Artificial neural networks (ANNs)

Artificial neural networks (ANNs) are a form of artificial intelligence, which, by means of their architecture, attempt is made to simulate the biological structure of the human brain and nervous system (Zurada, 1992; Fausett, 1994). A neural network consists of simple synchronous processing elements, called neurons, which are inspired by biological nerve system (Malinova and Guo, 2004). The mathematical model of a neural network comprises of a set of simple functions linked together by weights. The network consists of a set of input units x, output units y and hidden units z, which link the inputs to outputs. In this study, two different types of ANNs were developed. The first ANN model was multi-layer perceptron which is the most commonly-used neural network structure in ecological modeling and soil science (Agyare, 2007); whereas, the second ANN model was radial basis function. Matlab 7.1 software (2005) was used to develop PTFs for predicting CEC by means of ANN models.

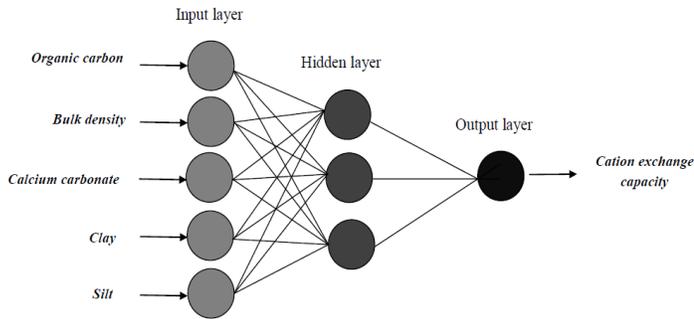
### Multi-layer perceptron (MLP)

Multi-Layer Perceptron has three layers including an input layer, one or more hidden layers and an output layer. Each layer has a number of processing units called neuron (node) and each unit is fully interconnected with weighted connections to units in the subsequent layer. The MLP

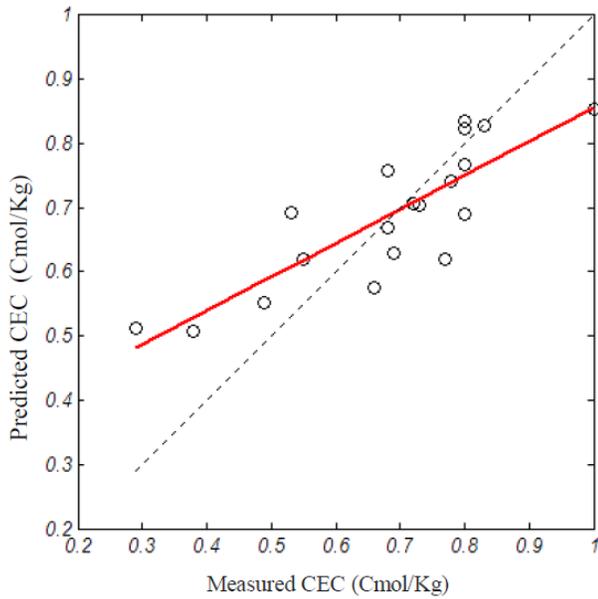
transforms n inputs to 1 from the first layer, which are transmitted through the hidden layer, to the output layer by means of some nonlinear functions. In order to find optimal weights by means of MLP, firstly the network is trained using a procedure called error back propagation by observing a large number of input and output examples to develop a useful formula for prediction. The output of the network is determined by the activation of the units in the output layer (Dawson et al, 2006; Yilmaz and Kaynar, 2011).

### Radial basis function (RBF)

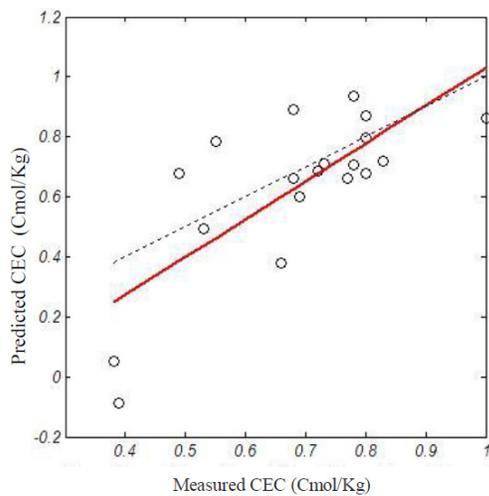
The structure of RBF is similar to that of MLP. The main difference between MLP and RBF is that, unlike the MLP, there is only a hidden layer in RBF network which contains nonlinear nodes called RBF units that measure the distance between an input data vector and the center of its RBF (Yilmaz et al, 2011). Training stage in RBF has two steps, firstly, calculating the function's center and its deviation or width and subsequently, calculating the output weights. There are various ways for selecting the centers and widths of functions such as random subset selection, K-means clustering, orthogonal least squares learning algorithm, and RBF-PLS. In this study, the forward subset selection routine was used to select the centers from training set samples. The adjustment of the connection weight between hidden layer and output layer is performed using a least squares solution



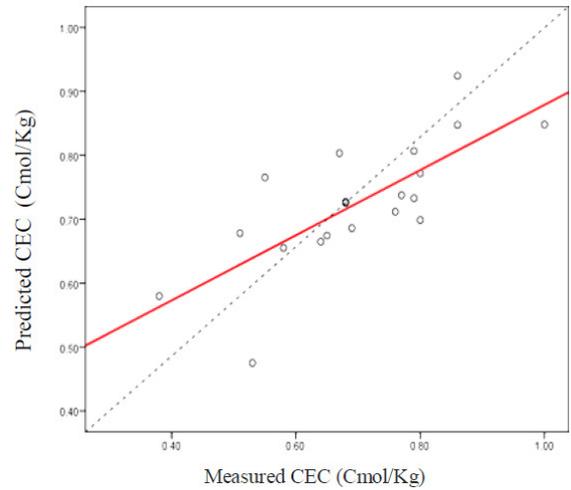
**Fig 3.** Structure of MLP and RBF networks for predicting CEC.



**Fig 4.** Measured versus predicted CEC values using MLP network.



**Fig 5.** Measured versus predicted CEC values using RBF network.



**Fig 6.** Measured CEC versus predicted CEC (Cmol/Kg) values using ANFIS.

after selecting the centers and width of radial basis functions (Yao, 2002; Yilmaz et al, 2011).

#### Adaptive neuro-fuzzy inference system (ANFIS) model

An adaptive network, as its name implies, is a network structure consisting of nodes and directional links through which the nodes are connected. Moreover, parts or all of the nodes are adaptive, which means each output of these nodes depends on the parameters pertaining to this node and the learning rule specifies how these parameters should be changed to minimize a prescribed error measure (Jange, 1993). In ANFIS, fuzzy rule bases are combined with neural networks to train the system using experimental data and obtain appropriate membership functions for process prediction and control (Lertworasirikul, 2008). Takagi–Sugeno–Kang (TSK) model (Takagi and Sugeno, 1985) that is one of the most frequently-used precise fuzzy models was used in the current study to predict soil CEC. In order to simplify, it is assumed that the inference system has two input variables  $x$  and  $y$  as each variable has two fuzzy subsets. A typical rule set with two fuzzy if–then rule set for a first-order Sugeno fuzzy model can be defined as Eq. 2 and 3:

$$\text{Rule 1: If } x \text{ is } A1 \text{ and } y \text{ is } B1 \quad \text{Then } f_1 = p_1x + q_1y + r_1 \quad (2)$$

$$\text{Rule 2: If } x \text{ is } A2 \text{ and } y \text{ is } B2 \quad \text{Then } f_2 = p_2x + q_2y + r_2 \quad (3)$$

Where  $A_1$ ,  $A_2$  and  $B_1$ ,  $B_2$  are the MFs for inputs  $x$  and  $y$  respectively,  $p_1$ ,  $q_1$ ,  $r_1$  and  $p_2$ ,  $q_2$ ,  $r_2$  are the parameters of the output function. The corresponding equivalent ANFIS architecture for two input variable first-order Sugeno fuzzy model with two rules is illustrated in Fig. 1(a). The general architecture of ANFIS consists of five layers, namely, a fuzzy layer, a product layer, a normalized layer, a defuzzy layer and a total output layer is depicted in Fig. 1(b). In this architecture, the circular nodes represent nodes that are fixed, whereas the square nodes are nodes that have parameters to be learnt.

Layer 1: Every node in this layer is represented by a square node including a node function. The node function employed

by each node determines the membership relation between the input and output functions.

Layer 2: every node in this layer is a fixed (circle) labeled II node and its output is produced by signals obtained from layer 1.

Layer 3: every node in this layer is a fixed (circle) node labeled N. The nodes normalize the firing strength by calculating the ratio of firing strength for this node to the sum of all the firing strengths.

Layer 4: Every node in this layer is represented by a square node including a node function.

Layer 5: The single node in this layer is a fixed (circle) node labeled  $\Sigma$  that computes the overall output as the summation of all incoming signals.

### Performance evaluation criteria

Two different types of standard statistical performance evaluation criteria were used to control the accuracy of the prediction capacity of the models developed. These are mean square error (MSE) and the determination coefficient ( $R^2$ ). The two performance evaluation criteria used in the current study can be calculated using Eq. 4 and 5:

$$R^2 = 1 - \frac{\sum_{i=1}^N (y_i - \hat{y}_i)^2}{\sum_{i=1}^N (y_i - \bar{y})^2} \quad (4)$$

$$MSE = \frac{1}{N} \sum_{i=1}^N (y_i - \hat{y}_i)^2 \quad (5)$$

Where N is the number of data,  $y_i$  is the measured value of each variable,  $\hat{y}_i$  is the predicted value of each variable and  $\bar{y}$  is the average of predicted value of each variable.

### Conclusion

In this study, an attempt has been made to analyze and compare multiple linear regressions (MLR), adaptive neuro-fuzzy inference system (ANFIS) and artificial neural network (ANN) including multi-layer perceptron (MLP) and radial basis function (RBF) models to develop pedo-transfer function for predicting soil cation exchange capacity by using available soil properties. The statistical prediction performances of used models are measured in terms of correlation coefficient ( $R^2$ ) and mean square error (MSE). The results of prediction CEC indicated that the measured correlation coefficient between predicted and observed data using equation obtained from the MLR and ANFIS models were approximately similar and very poor. The MLP model for prediction of CEC revealed the most reliable prediction when compared with the other models. Also, descriptive performance indices ( $R^2$  and MSE) between predicted and experimental data for RBF model showed higher accuracy comparing with both ANFIS and MLR models. Consequently, with the use of proposed ANNs especially, MLP network, the performance of CEC condensers can be determined by performing only a limited number of test operations, thus saving engineering effort, time and funds.

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