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Developing Pedotransfer Functions for Estimating Some Soil Properties using Artificial Neural Network and Multivariate Regression Approaches

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Abstract**—**Study of soil properties like field capacity (F.C.) and permanent wilting point (P.W.P.) play important roles in study of soil moisture retention curve. Although these parameters can be measured directly, their measurement is difficult and expensive. Pedotransfer functions (PTFs) provide an alternative by estimating soil parameters from more readily available soil data. In this investigation, 70 soil samples were collected from different horizons of 15 soil profiles located in the Ziaran region, Qazvin province, Iran. The data set was divided into two subsets for calibration (80%) and testing (20%) of the models and their normality were tested by Kolmogorov-Smirnov method. Both multivariate regression and artificial neural network (ANN) techniques were employed to develop the appropriate PTFs for predicting soil parameters using easily measurable characteristics of clay, silt, O.C, S.P, B.D and $CaCO_3$. The performance of the multivariate regression and ANN models was evaluated using an independent test data set. In order to evaluate the models, root mean square error (RMSE) and R^2 were used. The comparison of RSME for two mentioned models showed that the ANN model gives better estimates of F.C and P.W.P than the multivariate regression model. The value of RMSE and R^2 derived by ANN model for F.C and P.W.P were (2.35, 0.77) and (2.83, 0.72), respectively. The corresponding values for multivariate regression model were (4.46, 0.68) and (5.21, 0.64), respectively. Results showed that ANN with five neurons in hidden layer had better performance in predicting soil properties than multivariate regression.

Keywords**—**Artificial neural network, Field capacity, Permanent wilting point, Pedotransfer functions.

I. Introduction

FIELD capacity is defined as the maximum water content in a soil two to three days after being wetted and free drainage is negligible. Wilting point is defined as the soil water content where leaves of sunflower plants wilt continuously [7]. Soil water contents at field capacity and wilting point are used to calculate the water depth that should be applied by irrigation [9], and to determine water availability, which is a crucial factor in assessing the suitability of a land area for producing a given crop [36]. The development of models simulating soil processes has increased rapidly in recent years. These models have been developed to improve the understanding of important soil processes and also to act as tools for evaluating agricultural and environmental problems. Consequently, simulation models are now regularly used in research and management [22]. F.C, P.W.P and cation exchange capacity (CEC) are among the most important soil properties that are required in soil databases [18], and are used as inputs in soil and environmental models [1,15]. However, soil properties can be highly variable spatially and temporally, and measuring them is both time consuming and expensive. As a result, the most difficult and expensive step towards the process of environmental modeling is the collection of data. The term pedotransfer function (PTF) was coined by Bouma [5] as translating available data (those we have) into useful information (what we need). The most readily available data come from soil survey, such as field morphology, texture, structure and pH. Pedotransfer functions add value to this basic information by translating them into estimates of other more laborious and expensively determined soil properties. These functions fill the gap between the available soil data and the properties which are more useful or required for a particular model or quality assessment.

The two common methodologies used to develop PTFs are multiple-linear regression (MLR) and artificial neural network (ANN) modeling techniques. 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 [40]. A more advanced approach to model PTFs is to make use of ANN technique [33]. ANN offers a fundamentally different approach for modeling soil behavior. ANN is an oversimplified simulation of the human brain and is composed of simple processing units referred to as neurons. It is able to learn and generalize from experimental data even if they are noisy, imperfect or non-linear in nature. This ability allows this computational system to learn constitutive relationships of materials directly from the result of experiments. Unlike conventional models, it needs no prior knowledge, or any constants and/or assumptions about the deformation characteristics of the geomaterials. Other powerful attributes of ANN models are their flexibility and adaptivity, which play important roles in material modeling. When a new set of experimental results cannot be reproduced by conventional models, a new constitutive model or a set of new constitutive equations needs to be developed. However, trained ANN

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models can be further trained with the new data set to gain the required additional information needed to reproduce the new experimental results. These features ascertain the ANN model to be an objective model that can truly represent natural neural connections among variables, rather than a subjective model, which assumes variables obeying a set of predefined relations [3]. In brief, a neural network consists of an input, a hidden, and an output layer all containing "nodes". The number of nodes in input (e.g. soil bulk density, soil particle size data and etc) and output (different soil properties) layers are usually fixed, i.e., correspond to the number of input and output variables of the model [19]. A type of ANN known as multilayer perceptron (MLP), which uses a back-propagation training algorithm, is usually used for generating PTFs [1,22,23,33]. This network uses neurons whose output is a function of a weighted sum of the inputs. The major advantage of neural networks over the two groups of PTFs described earlier is that they do not require a-priori knowledge of the relations between input and output data [32]. However, because of their greater feasibility, ANN models are generally expected to be superior to MLR models [1,23,31]. Many studies related to modeling various soil parameters using different types of PTFs has been conducted. Schaap et al. [33] developed some functions for estimation of the different parameters of van Genuchten, van Genuchten-moalem, and Gardner equations by means of ANNs. Their results showed that with increasing the number of input data, the accuracy of functions would enhance. Omid et al. [26] adapted ANN to model sequent depth and jump length, both important parameters in the design of stilling basins with hydraulic jumps. 16 configurations, each with different number of hidden layers and/or neurons, were evaluated. The optimal models were capable of predicting sequent depth and jump length for a wide range of conditions with a mean square error (MSE) of 10%. A comparative study among MFNN and empirical models was also carried out. They found ANN models performed superior than regression models. Vos et al. [39] used 12 PTFs and Brazilian's database for prediction of bulk density. Their results showed that the separation of subsoil data from topsoil data did not increase the accuracy of prediction. Similarly, Heusher et al. [10] and Kaur et al. [14] reported that the soil texture and organic matter content were the main parameters for estimating of bulk density. Najafi and Givi [24] used the ANNs and PTFs methods for prediction of soil bulk density. They pointed out that the ANNs are able to predict the soil bulk density better than the PTFs. Amini et al. [1] estimated the cation exchange capacity (CEC) in the central of Iran using soil organic matter and clay content. They used the ANN and five experimental models that were on the basis of regression methods for their predictions. They showed that a neural network PTF with eight hidden neurons was able to predict CEC better than the regression PTFs. Also the ANN model significantly improved the accuracy of the prediction by up to 25%. They concluded that network models are in general more suitable for capturing the non-linearity of the relationship between variables. Jain and Kumar [12] indicated that the ANN technique can be successfully employed for the purpose of calibration of infiltration equations. They had also found that the ANNs are capable of performing very well in situations of limited data availability. In contrast Merdun et al. [20] pointed out that although the differences between regression and ANN models were not statistically significant, regression predicted point and parametric variables of soil hydraulic parameters better than ANN. The present study was carried out with an objective of comparing the ability of ANNs and multivariate regression for estimating F.C and P.W.P using some easily measurable soil parameters in Ziaran region of Qazvin province, Iran.

II. Materials and methods

Study area: The land investigated in the research is located in Ziaran (Qazvin province in Iran) which has an area about 5121 hectares; between latitudes of 35°58´ and 36°4´ N and longitudes of 50°24´ and 50°27´ E. The average, minimum and maximum heights points of Ziaran district are 1204, 1139 and 1269 meters from the sea level, respectively. Figure 1 shows the study area in Iran. The soil moisture and temperature regimes of the region by means of Newhall software are Weak Aridic and Thermic, respectively. Based on soil taxonomy [38], this region has soils in Entisols and Aridisols orders.

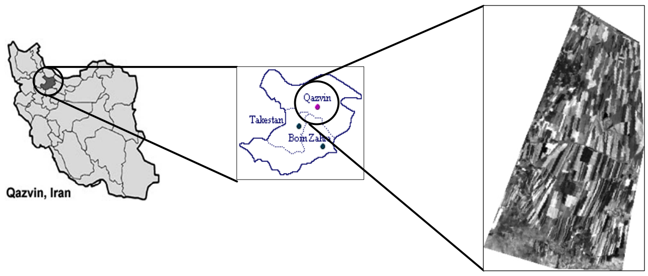

Fig. 1 Location of the study area

Data collection and soil sample analysis: After preliminary studies of topographic maps (1:25000), using GPS, studying location was appointed. 70 soil samples were collected from different horizons of 15 soil profiles (Fig. 1). Measured soil parameters included texture (determined using Bouyoucos hydrometer method), and organic carbon (determined using Walkley-Black method) [27]. The clod method [4] was used to determine bulk density (B.D). The moisture contents at field capacity and wilting point were determined with a pressure plate apparatus at -33 and -1500 kPa, respectively [6]. Water saturation percentage (SP) and $CaCO_3$ content were determined using gravimetery and Calcimetry methods, respectively [35].

III. Methods to fit PTFs

Multivariate regression: The most common method used in estimation PTFs is to employ multiple linear regressions. For example:

$$Y = aX_1 + bX_2 + cX_3 + ... \qquad (1)$$

Where: Y denotes depended variable, X_i ($i = 1,2.\cdots,n$) is independent variable, and a, b, … are unknown coefficients of the model.

Artificial neural network: Neural classifiers can deal with numerous multivariable nonlinear problems, for which an accurate analytical solution is difficult to obtain [30]. An artificial neural network is a highly interconnected network of many simple processing units called neurons, which are analogous to the biological neurons in the human brain. Neurons having similar characteristics in an ANN are arranged in groups called layers. The neurons in one layer are connected to those in the adjacent layers, but not to those in the same layer. The strength of connection between the two neurons in adjacent layers is represented by what is known as a 'connection strength' or 'weight'. An ANN normally consists of three layers, an input layer, a hidden layer, and an output layer. In a feed forward network, the weighted connections feed activations only in the forward direction from an input layer to the output layer. On the other hand, in a recurrent network additional weighted connections are used to feed previous activations back into the network. The structure of a feed-forward ANN is shown in Figure 2. This ANN is a popular neural network which known as the back propagation algorithm introduced by Karaca and Ozkaya [13]. This ANN had k input and one output parameters. They used this ANN for accurate modeling of the leachate flow-rate. They also reported that the input parameters, number of neurons at the hidden and output layer should be determined according to currently gathered data. Moreover, an important step in developing an ANN model is the training of its weight matrix. The weights are initialized randomly between suitable ranges, and then updated using certain training mechanism [23,28,33]. In the feed-forward networks, error minimization can be obtained by a number of procedures including Gradient Descent (GD), Levenberg–Marquardt (LM) and Conjugate Gradient (CG). BP uses a gradient descent (GD) technique which is very stable when a small learning rate is used, but has slow convergence properties [27]. Several methods for speeding up BP have been used including adding a momentum term or using a variable learning rate. In this study, LM algorithm in the sense that a momentum term is used to speeding up learning and stabilizing convergence is used.

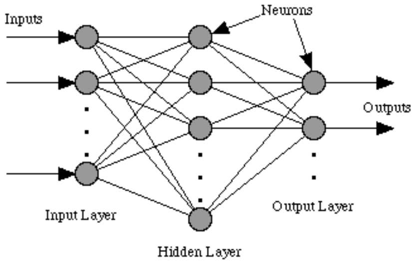

Fig. 2 Structure of feed-forward ANN

Performance criteria: The performance of the models was evaluated by a set of test data using the root mean square error (RMSE) and the coefficient of determination (R^2) between predicted and measured values. The RMSE is a measure of accuracy and reliability for calibration and test data sets [41] and is defined as:

$$RMSE = \sqrt{\frac{1}{n}\sum_{k=1}^{n}(z_o - z_p)^2} \qquad (2)$$

Where: Z_o is observed value, Z_p is predicted value, n is number of samples.

NeuroSolutions 5.0 software was used for the design and testing of ANN models. Data were subdivided into two sets: 80% for training the networks and the remaining 20% for testing purposes. Soil parameters including clay, silt, O.C, CaCO3, SP and B.D were input data for prediction of the two outputs (F.C and P.W.P.). In this study, the ANN structures were all consisted of one hidden layer, a sigmoid activation function in hidden layer, and a linear activation function in output layer and LM algorithm was used to train the networks due to efficiency, simplicity and high speed. To develop a statistically sound model, the networks were trained three times and the best values were recorded for each parameter [27]. To avoid "overfitting", the MSE of the CV subset was calculated after adjusting of weights and biases. The training process continued until the minimum MSE of the validating sets was reached (early-stopping scheme). The network weights and biases are then adapted and employed for validation in order to determine the neural network model overall performance. The RMSE and R^2 of the ANN models on test sets are then calculated and compared with multivariate regression model.

IV. Results and Discussion

Data summary statistics: Data summary of training and testing sets are presented in Tables I and II, respectively.

TABLE I

Statistics of training data sets for F.C and P.W.P

	Soil parameter	Min	Max	Mean	Std
Training set	Clay (%)	4.40	55.60	22.30	11.83
	Silt (%)	2.80	62.80	30.10	12.86
	O.C (%)	0.04	1.10	0.35	0.23
	$CaCO_3$ (%)	2.86	25.4	10.63	5.92
	SP (%)	21.18	65.67	34.76	9.26
	B.D ($g.cm^{-3}$)	1.20	1.71	1.50	0.11
	F.C (%)	10.80	32.50	17.38	4.65
	P.W.P (%)	5.72	16.40	9.02	2.36

TABLE II
STATISTICS OF TESTING DATA SETS FOR F.C. AND P.W.P

	Soil parameter	Min	Max	Mean	Std
Testing set	Clay (%)	17.20	54.80	29.99	10.49
	Silt (%)	6.00	40.80	22.44	11.58
	O.C (%)	0.19	0.66	0.38	0.13
	$CaCO_3$ (%)	11.00	30.20	17.32	5.01
	SP (%)	28.62	59.51	39.07	9.61
	B.D ($g.cm^{-3}$)	1.26	1.70	1.46	0.13
	F.C (%)	14.40	29.62	19.61	4.81
	P.W.P (%)	6.81	15.20	9.96	2.63

Simple linear correlation coefficients (r) among F.C., P.W.P. and independent variables were also calculated (Table III). As Table III illustrates correlations among SP, clay and F.C. and also, among SP, clay and P.W.P. were positive and highly significant. For example the correlation coefficients between F.C and clay content (r = 0.75) is rather similar to the between P.W.P and clay content (r = 0.71).

Also, the correlation coefficient between B.D and O.C content (r = -0.58) is rather more than between B.D and S.P (r = -0.27). However with regarding to these correlation coefficients, both of them are suitable for developing PTFs for prediction of F.C and P.W.P in soils of Ziaran region. Similarly these correlations between F.C and SP (r = 0.95) and also, between P.W.P and SP (r = 0.90) were positive and significant. The correlation between $CaCO_3$ and clay content (r = 0.59) and between $CaCO_3$ and SP (r = 0.49) were relatively high. In addition with regarding to this table it is clear that B.D is negatively correlated with F.C (r = -0.29) and P.W.P (r = -0.23). Hence with respecting to Table III, multivariate regression equations were developed for studied parameters using SPSS 15 software. We selected only regression model that had a coefficient of determination (R^2), greater than 0.5 [1,17]. These equations were expressed as:

$$F.C. = 3.484 - 0.003\,Clay + 0.027\,Silt - 1.3\,O.C - 0.005\,CaCO_3 + 0.48\,SP - 2.15\,B.D \quad , \quad R^2 = 0.68 \qquad (3)$$

$$P.W.P. = 2.779 + 0.006Clay + 0.016Silt - 1.36O.C - 0.036CaCO_3 + 0.24SP - 1.38B.D \quad , \quad R^2 = 0.64 \qquad (4)$$

TABLE III
SIMPLE LINEAR CORRELATION COEFFICIENTS (R) AMONG F.C, P.W.P AND INDEPENDENT VARIABLES

	Clay (%)	Silt (%)	O.C (%)	$CaCO_3$ (%)	SP (%)	B.D ($g.cm^{-3}$)	F.C (%)	P.W.P (%)
Clay (%)	1							
Silt (%)	0.19	1						
O.C (%)	0.09*	0.28*	1					
$CaCO_3$ (%)	0.59**	-0.01	-0.14	1				
SP (%)	0.76**	0.26*	0.18	0.49**	1			
B.D ($g.cm^{-3}$)	-0.22	0.05	-0.58**	-0.03	-0.27*	1		
F.C (%)	0.75**	0.28*	0.16	0.52**	0.95**	-0.29*	1	
P.W.P (%)	0.71**	0.31*	0.13	0.45**	0.90**	-0.23*	0.88**	1

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

After determining of Eqs.(3) and (4), performance of multivariate regression was developed for test data set . Coefficient of determination (R^2) and RMSE for F.C. and P.W.P. have been obtained 0.68, 4.46 and 0.64, 5.21 respectively. Sarmadian et al. [31] also observed similar correlation coefficient in their results for F.C. (r = 0.75) and P.W.P. (r = 0.66).

Developing PTFs using multivariate regression and artificial neural network: After For predicting the soil F.C. and P.W.P. by means of ANNs, the input feature vector was similar to those used for multivariate linear regression. In the present study for predicting soil properties we did not increase the input data for constructing ANN, because according to findings of Lake et al. [17] and Amini et al. [1] increasing the number of inputs will decrease the accuracy of the estimations. For example for predicting a soil characteristics if just one types of the input data have low correlation coefficients with output data, the accuracy of the model will automatically decrease. Therefore the ANN input layer was consisted of six data in this model were consisted of exploratory variables, namely, clay, silt, O.C, $CaCO_3$, SP and B.D After randomizing and splitting of data set into training and testing data, various ANN structures of the topology 6-k-2, i.e., networks having six neurons in the input layer, one hidden layer with different number or neuron (k=1, 2, …,10), and two neurons (F.C and P.W.P) as the output layer were designed. The optimum structures of network were decided by means of R^2 and RMSE criteria. The RMSE values for various k (numbers of neurons in the hidden layer) related to studied soil parameters are presented in the Figures 3 and 4. As shown in this figures, the minimum level of RMSE for F.C. and P.W.P is related to the network having five neurons in the hidden layer. Also, with regarding to this figures can be realize that with increasing the number of neurons, the overall efficiency of models will decrease and hence, the best performance is related to the networks having optimum numbers of neurons, i.e. the 6-5-2-MLP. The levels of RMSE and R^2 for F.C. and P.W.P. were 2.35, 0.77 and 2.83, 0.72 respectively. In addition, the levels of R^2 (and RMSE) derived by ANN for studied soil parameters had higher (and lower) values than those derived by multivariate linear regression (Table IV) which is in line with the work done by Sarmadian et al. [31], Amini et al. [1], Tamari et al. [37], Minasny and McBratney [22] and Schaap et al. [33].

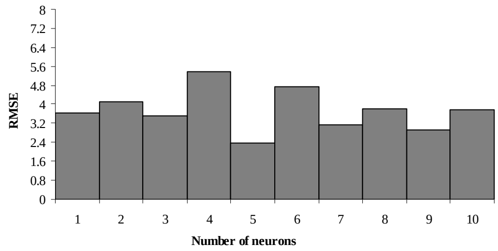

Fig. 3 RMSE values for 1-10 neurons in hidden layer (F.C)

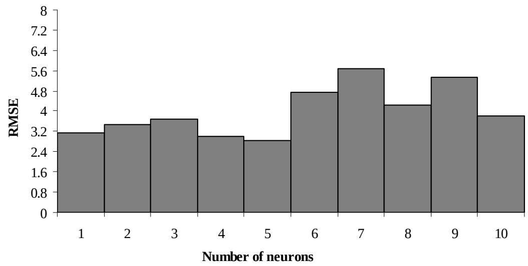

Fig. 4 RMSE values for 1-10 neurons in hidden layer (P.W.P)

Schaap et al. [33] confirmed applicability of ANNs and concluded that accuracy of these models depend on the number of inputs. Amini et al. [1] found that the neural network-based models provided more reliable predictions than the regression-based PTFs. Koekkoek and Booltink [16] found that ANN performed slightly better, but the differences were not significant. The network models for F.C and P.W.P were more suitable for capturing the non-linearity of the relationship between variables. One of the advantages of neural networks compared to traditional regression PTFs is that they do not require a priori regression model, which relates input and output data and in general is difficult to guess because these models are not known [32,33].

The scatter plot of the measured against predicted F.C and P.W.P for the test data set are given in Figures 5 and 6 for the ANN model which we identified as being the best model for predicting soil parameters. So that according to these diagrams, the best fitted line has the angle of near to 45° that shows the high accuracy of estimation by the ANN model.

TABLE IV
CALCULATED STATISTICAL PARAMETERS IN TEST STAGE FOR DIFFERENT METHODS BASED ON PEDOTRANSFER FUNCTIONS

Statistical parameters	Multivariate linear regression (F.C)	Multivariate linear regression (P.W.P)	Artificial neural network (F.C)	Artificial neural network (P.W.P)
RMSE	4.46	5.21	2.35	2.83
R^2	0.68	0.64	0.77	0.72

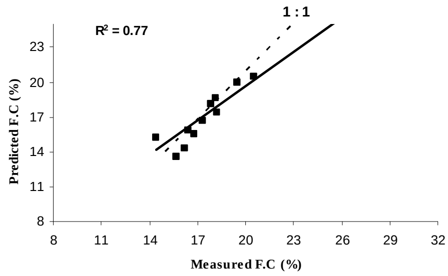

Fig. 5 The scatter plot of the measured versus predicted F.C

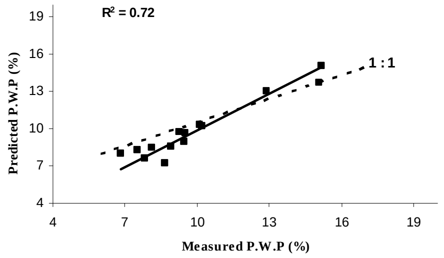

Fig. 6 The scatter plot of the measured versus predicted P.W.P

The reason of this superior efficiency of ANNs models compared with the basic regression equations are probably because; the PTFs that have been derived from various areas have different efficiencies. On the other hand, according to the hypothesis of Schaap et al. [33], for designing of a neural network we do not need a special equation. However, they believe that with creation of a suitable equation between input and output data we are able to achieve to the best results. Also, due to the inherent nonlinearity between the exploratory variables and predicting variables, the neural networks have the better efficiency compared with the basic regression equations. Pachepsky et al. [28] investigated the accuracy of ANN and analyzed the regression method using correlation coefficient and the RMSE. They reported that the neural network is able to predict the easily measurable soil parameters with more accuracy and less error. Similar results have been reported by the Tamari et al. [37] as well. They found that using ANN leads to less RMSE values than the multivariable linear regression. They also reported that the neural network has not better efficiency than linear regression models in occasion of high stability of data. However, the high accuracy of data leads to more efficiency of neural network and also, shows the proper selection of testing and training data. Analysis of the ANN parameters suggested that more input variables were necessary to improve the prediction of soil parameters [21,37]. As Figures 5 and 6 showed ANN predicted soil properties with relatively high accuracy (R^2 = 0.77 and 0.72). In practice, it is extremely difficult to saturate a soil with water because of air trapping [11,21]. Tamari et al. [37] predicted poorly K values at matric potentials of -10 and -25 kPa with both methods of ANN and regression, and they suggested that soil samples should be classified based on their texture as coarse, medium and fine. Therefore, difficulty in measuring soil hydraulic properties in heterogeneous soils might cause this relatively poor prediction. Analysis of the ANN parameters suggested that more input variables were necessary to improve the prediction of unsaturated hydraulic conductivity [21,37]. The differences between the field and laboratory determination of water retention data might be associated to the insufficient representation of large pores in the laboratory, sample disturbance and spatial variation, hysteresis, and scale effects related to the sample size [8,21,34]. Pachepsky and Rawls [29] found significant differences between the field and laboratory volumetric water contents for coarse-, intermediate-, and fine-textured soil horizons. Therefore, measurement errors might cause poor prediction of the parameters.

V. Conclusion

In this study, multivariate linear regression and neural network model (feed-forward back-propagation network) were employed to develop a pedotransfer function for predicting soil F.C and P.W.P by using available soil properties. For predicting the soil property by means of PTFs, the input data were consisted of clay, silt, O.C, $CaCO_3$, SP and B.D for F.C and P.W.P The performance of the multivariate linear regression and neural network model was evaluated using a test data set. Results showed that ANN with five neurons in hidden layer had better performance in predicting soil F.C and P.W.P than multivariate regression. The network model for these parameters was more suitable for capturing the non-linearity of the relationship between variables. ANN can model non-linear functions and have been shown to perform better than linear regression.

With regarding to the evaluation criteria, the results of this study revealed that ANNs had superiority to the basic regression equations for prediction of mentioned soil parameters. This is a crucial result, since ANN– PTFs formed from local data produce more accurate predictions than those built from data spread from a wider area, the concept of data conservation becomes a critical factor in ANN–PTF construction [2]. However, due to difficulties of direct measurement of soil parameters, we recommend using of neuro-fuzzy models such as ANFIS in the future studies for obtaining the logical equations of other soil parameters, especially soil hydraulic properties, in each area. ANFIS is more tolerant to noisy or missing data, and has a good generalization capability. ANN posses a number of properties for modeling PTFs: universal function approximation capability, learning from experimental data, tolerance to noisy or missing data, and good generalization capability. When function approximation is the goal, the ANN model will often deliver close to the best fit. The present work was motivated in this direction. Apart from model accuracy and generalization capability, other important issues such as computational time, credibility, tactical issues and replicating the results have to be considered when comparing multivariate linear regression vs. ANN to predict soil F.C and P.W.P Although outperforming the empirical modeling techniques, ANN has one big offset - it is hard to draw any physical information out of it, i.e. no information from the neurons' weights and biases can be drawn about the weights of each predictor in the final score [27]. Nevertheless, because of their better results, ANNs are commonly used during the past 10 years to solve non-linear problems of high complexity.

Acknowledgment

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