Computers and Electronics in Agriculture 92 (2013) 92–103

Contents lists available at SciVerse ScienceDirect

Computers and Electronics in Agriculture

journal homepage: www.elsevier.com/locate/compag

Combination of artificial neural networks and fractal theory to predict soil water retention curve

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ARTICLE INFO

Article history:
Received 1 September 2012
Received in revised form 10 January 2013
Accepted 12 January 2013

Keywords:
Aggregate size distribution
Artificial neural networks
Fractal parameters
Particle size distribution
Pedotransfer functions
Water retention

ABSTRACT

Despite good progress in developing pedotransfer functions (PTFs), the input variables that are more preferable in a PTF have not been yet determined clearly. Among the modeling techniques to characterize soil structure, those using fractal theory are in majority. For the first time, fractal parameters were used as predictors to estimate the water content at different matric suctions using artificial neural networks (ANNs). PTFs were developed to estimate soil water retention curve (SWRC) from a dataset of 148 soil samples from North West of Iran. Including geometric mean (d_g), geometric standard deviation (s_g), and median diameter (M_d) of particle size distribution as input parameters significantly enhanced the PTFs' accuracy and increased the coefficient of determination (R^2) by up to 5.5%. Fractal parameters of particle size distribution (PSDFPs) were used as predictors and it improved the accuracy and reliability by decreasing root mean square error (RMSE) by up to 30% for water content at h value of 5 kPa ($\theta_{5\ \mathrm{kPa}}$) and by up to 12.5% for water content at h value of 50 kPa ($\theta_{50\ \mathrm{kPa}}$). Entering the fractal parameters of aggregate size distribution (ASDFPs) in the models raised the accuracy at most soil matric suctions (h) and caused up to 6.7% reduction in the RMSE. Their impacts were significant at $\theta_{25\ \mathrm{kPa}}$ and $\theta_{50\ \mathrm{kPa}}$. The network architectures were unique and problem specific with respect to the output layer transfer functions and number of hidden neurons. Adding PSDFPs and ASDFPs to the input parameters of the proper ANN models could improve the estimation of SWRC, significantly.

1. Introduction

Knowing the soil hydraulic properties is needed for many applications in hydrology, agronomy, meteorology, ecology, environmental protection (Tomasella et al., 2003) and developing water and solute flow models (Pan et al., 2012). Perhaps the most fundamental soil hydraulic property is the soil water retention characteristic. Direct measurements of these properties are highly costly, time consuming and sometimes it is not possible to measure them for large scale environmental impact studies (Nemes et al., 2009).

Therefore, attempts have been made to develop pedotransfer functions (PTFs) to estimate soil hydraulic properties from more easily-available soil data, such as texture, organic matter, bulk density (Gupta and Larson, 1979), saturated hydraulic conductivity (Vereecken et al., 1992), soil genetic information (Tietje and Tapkenhinrichs, 1993), type of soil horizon (Al Majou et al., 2008) structure (Koekkoek and Booltink, 1999), cation exchange capacity (Pachepsky and Rawls, 1999), geometric mean and standard deviation of particles diameter, d_g and s_g (Scheinost et al., 1997), cone index (CI; Pachepsky et al., 1998), effective porosity (Schaap et al., 1998), specific surface area (Walczak et al., 2004), geometric specific surface area (Walczak et al., 2006), topography and vegetation attributes (Sharma et al., 2006), soil type (Rab et al., 2011) and remotely sensed data such as elevation and leaf area index (Jana and Mohanty, 2011).

Kutlu1 and Ersahin (2008) evaluated the performance of ROSETTA program in the estimation of the van Genuchten water retention model parameters using regression technique and reported that general performance of ROSETTA was low for α but did better estimation for n. In addition, they reported that the prediction errors of ROSETTA are large. However, Das and Verma (2011) concluded that the point estimation of soil moisture could be

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0168-1699/$ - see front matter
http://dx.doi.org/10.1016/j.compag.2013.01.005

Nomenclature

AIC	Akaike information criterion	MLP	multilayer perceptron
A_R	intercept of Rieu and Sposito's model	NHN	number of hidden neurons
BD	bulk density	OLTF	output layer transfer function
C	clay	RMSE	root mean square error
c_{Bi}	intercept of Bird's model	R^2	coefficient of determination
c_{1M}	intercept of first domain of Millan's model	S	sand
c_{2M}	intercept of second domain of Millan's model	Se_B^2	variance of mass of aggregates for Bartoli's model
D_{Bi}	mass fractal dimension of Bird's model	Se_{Bi}^2	variance of cumulative mass of particles for Bird's model
$d_{c\ M}$	critical particle size, separating the two domains in Millan's model	Se_M^2	variance of cumulative mass of particles for Millan's model
d_g	geometric mean of particle diameter	Se_R^2	variance of cumulative number of aggregates for Rieu and Sposito's model
D_{mB}	mass fractal dimension of Bartoli's model	Se_T^2	variance of the ratio of cumulative mass of particles to total mass for Tyler and Wheatcraft's model
D_{mT}	mass fractal dimension of Tyler and Wheatcraft's model	Se_B^Y	variance of the ratio of cumulative mass to total mass of particles for Yang's model
D_{mY}	mass fractal dimension of Yang's model	s_g	geometric standard deviation of particle diameter
D_{nR}	fragmentation fractal dimension of Rieu and Sposito's model	Si	silt
D_{1M}	fractal dimension of first domain in Millan's model	TP	total porosity
D_{2M}	fractal dimension of second domain in Millan's model	θ	gravimetric water content
GMER	geometric mean error ratio		
GSDER	geometric standard deviation of the error ratio		
k_{mB}	intercept of Bartoli's model		
M_d	median diameter		
MGN	Morgan–Granger–Newbold		

generated from texture and bulk density, but they did not report coefficients of determination larger than 0.62. Khodaverdiloo et al. (2011) by developing PTFs for some calcareous soils found that $CaCO_3$ did not affect the accuracy of the PTFs in the prediction of soil water retention curve (SWRC). Tóth et al. (2012) used $CaCO_3$ and soluble salt contents, pH, and soil subtype classes to predict SWRC for salt affected soils.

Despite the diverse parameters which have been employed in developing PTFs, one basic question still remained unanswered: which input variables are preferable or necessary to be included in a PTF (Wösten et al., 2001)? In other words, the question is whether new input variables can be found to improve the performance of PTFs or not.

Among all of the available modeling techniques to characterize the soil structure, those utilizing fractal theory are in the majority. An appropriate use of fractals can lead to rigorous quantification of the heterogeneity, tortuosity, and connectivity of the soil pore/solid space, or the power-law distribution of number sizes produced from fragmentation process (Tyler and Wheatcraft, 1990; Bartoli et al., 1991; Perfect and Kay, 1991; Rasiah et al., 1992; Crawford et al., 1993; Bird et al., 2009; Gregory et al., 2012). Fractal theory has been employed to explain the processes of water retention and movement in soil (Tyler and Wheatcraft, 1990; Rieu and Sposito, 1991; Crawford et al., 1995). Tyler and Wheatcraft (1990) and Crawford et al. (1995) produced relatively simple fractal models to explain the power-law exponent in the Brooks–Corey model for soil water retention. The important outcome was that the previously empirical exponent now got a physical relevance and could be determined by a fractal model. Xu and Dong (2004) used the fractal dimension of pore size distribution to obtain SWRC, unsaturated hydraulic conductivity, and water diffusivity functions. Recently, Bayat et al. (2011) successfully used fractal parameters to estimate Brooks and Corey (1964) parameters using artificial neural networks (ANNs) and multi-objective group method of data handling. In soil science, ANNs have been successfully used to predict water retention characteristics from other, more easily measured, soil variables like particle size distribution and bulk density (Schaap et al., 2001; Sharma et al., 2006). Vereecken et al. (2010) proposed establishment of databases of soil hydraulic properties that contain new predictors such as soil structural properties. They suggested that successful use of structural properties in PTFs will require parameterizations that account for the effect of structural properties on soil hydraulic functions. In this regard, aggregate size distribution can be a good index for soil structure. Then, fitting a suitable fractal model to the aggregate size distribution data and using its parameters to predict SWRC would be a step forward in developing PTFs.

Artificial neural network (ANN) is a powerful technique that has received great attentions to predict the SWRC (Pachepsky et al., 1996; Schaap and Bouten, 1996; Schaap et al., 1998; Koekkoek and Booltink, 1999). Also, ANN was used to predict other soil parameters such as electrical conductivity (Namdar-Khojasteh et al., 2010) and cation exchange capacity (Amini et al., 2005). However, it is important to match the neural architecture and the hidden layer and output layer transfer functions to a specific problem (NeuroSolutions, 2005). The number of hidden neurons depends on the complexity of the underlying problem. It is determined empirically by calibrating neural networks with different number of hidden neurons (Schaap et al., 1998). Nevertheless, most researchers use only multilayer perceptrons (MLPs) with specific hidden layer transfer functions, output layer transfer functions, and number of hidden neurons to estimate the SWRC (Pachepsky et al., 1996; Schaap and Bouten, 1996; Schaap et al., 1998; Koekkoek and Booltink, 1999; Minasny et al., 1999; Schaap et al., 2001; Minasny and McBratney, 2002; Minasny et al., 2004; Sharma et al., 2006). Using only one ANN type with specific architecture limits the ANN capability in prediction. Khodaverdiloo et al. (2011) reported better accuracy of regression-based PTFs when compared with the ANN-based PTFs of ROSETTA. Twarakavi et al. (2009) also reported poor results of ANN model. They used support vector machines to derive a new set of PTFs and found that all the support vector machines-based PTFs performed better than the ROSETTA PTF program. The reason could be attributed to the use of only one ANN type with specific architecture. ANN has a high flexibility in architecture and structure.

Other types of ANNs, such as general regression neural networks, have also been used by Tamari et al. (1996) and Amini et al. (2005) to predict saturated hydraulic conductivity (K_s) and