Canadian Geotechnical Journal

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Journal:	<i>Canadian Geotechnical Journal</i>
Manuscript ID	cgj-2020-0562.R1
Manuscript Type:	Article
Date Submitted by the Author:	16-Jan-2021
Complete List of Authors:	Li, Yao; University of Ottawa Vanapalli, Sai; University of Ottawa, Civil Engineering
Keyword:	Soil-water characteristic curve, grain-size distribution, artificial neural network, multivariate adaptive regression splines, AI aid design method
Is the invited manuscript for consideration in a Special Issue? :	Not applicable (regular submission)

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**Prediction of Soil-Water Characteristic Curves using two Artificial Intelligent
(AI) Models and AI Aid Design Method for Sands**

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**Technical Article Revised and Submitted to
Canadian Geotechnical Journal for Review and Publication
15th Jan. 2020**

ABSTRACT

In this paper, two artificial intelligent models (i.e., artificial neural networks (ANN) and multivariate adaptive regression splines (MARS)) were developed using cumulative percentiles from grain-size distribution (GSD) curve as input information to predict the soil-water characteristic curve (SWCC). The importance of each input variable was testified using two different sensitivity analyses. The results show a strong correlation between the SWCC and GSD curves based on large volume of datasets. The ANN provides higher accuracy due to its unique structure; however, MARS model facilitates in developing a regression equation that contributes to stable performance. The SWCC can be reliably predicted with MARS regression equation using one data point from the GSD curve and bulk density information. Sensitivity analysis suggests that the prediction of the SWCC is also possible with a reasonable degree of accuracy by using single data point information from the GSD curve as an input variable. Finally, a novel AI aid design method is proposed by combining MARS regression equation along with physico-empirical model and fitting equation that provides a rapid and reliable technique for predicting the SWCC of sands.

No. of words in the abstract: 181

Keywords: *Soil-water characteristic curve, grain-size distribution, artificial neural network, multivariate adaptive regression splines; AI aid design method*

INTRODUCTION

The relationship between water content (i.e., gravimetric or volumetric) or degree of saturation and matric suction is widely referred to as the soil-water characteristic curve (SWCC) in the literature. The terms soil moisture curve (SMC) and soil-water retention curve (SWRC) are also used in describing this relationship (Fredlund and Rahardjo 1993). Many models are proposed in the literature to fit the SWCC (e.g., Gardner 1958, van Genuchten 1980, Fredlund and Xing 1994). During the last 25 years, there has been a significant interest to predict the variation of hydro-mechanical properties of unsaturated soils using the SWCC as a tool in the geotechnical and geo-environmental engineering fields (e.g., Fredlund et al. 1994, Vanapalli et al. 1996, Sun et al. 2007, Cui et al. 2008, Alsherif and McCartney 2015, Yin and Vanapalli 2018). Significant advances were made in the literature towards designing infrastructure such as the retaining walls, pavements, slopes, shallow and deep foundations for unsaturated soils (e.g., Vanapalli 2009, Zhan et al. 2012, Zhang et al. 2014, Oh and Lu 2015, Qi and Vanapalli 2015, Shahrokhbabadi et al. 2019, Mahmoudabadi and Ravichandran 2020), using the SWCC as a tool, in recent years. However, there is lack of simple and inexpensive technique for rapid and reliable estimation or prediction of the SWCC (Alowaisy et al. 2020). This is one of the limitations towards extending the state-of-the-art understanding of the mechanics of unsaturated soils into engineering practice applications.

There were some attempts in the literature to predict or estimate the SWCC from GSD curves due to similarities between the SWCC and GSD curves. One of the widely used methods is based on scaling factor and pore shapes of soils to build a physicoempirical model (Arya and Paris (1981)). Following this method, various other models with scaling factors have been proposed in the literature (e.g., Tyler and Wheatcraft 1989, Zhai et al. 2020, Alves et al. 2020). Other methods include statistical estimation (Saxton et al. 1986, Vereecken et al. 1989, Fredlund et al. 2002, Chiu et al. 2012), correlation of soil properties with parameters of fitting

models (Perera et al. 2005, Vanapalli and Catana 2005, Chin et al. 2010, Chai and Khaimook 2020) and artificial intelligent (AI) evaluation (Pachepsky et al. 1996, Schaap and Bouten 1996, Schaap and Leij 1998, Koekkoek and Booltink 1999, Minasny and McBratney 2002, Johari et al. 2006). Table 1 summarizes five equations (i.e., eqs. 1 through 5) that are widely used models.

Various AI models have been successfully developed for geotechnical engineering applications during the last decade (e.g., Ren et al. 2019, Jin and Yin 2020, Zhang et al. 2020). There has been interest for predicting the SWCC from AI methods (e.g., Jain et al. 2004, Moreira de Melo and Pedrollo 2015) because of its wide use in interpretation of the hydro-mechanical behavior of unsaturated soils (e.g., Fredlund et al. 1994, Vanapalli et al. 1999, Chiu and Ng 2012, Tripathy et al. 2014, Burton et al. 2020). However, only a few studies have been undertaken in the literature to predict the SWCC directly from GSD curves using AI models (D'Emilio et al. 2018, Amanabadi et al. 2019). The focus of these studies was directed to predict the SWCC using clay, silt, and sand content information from the database. There is an urgent need for simple yet reliable methods for predicting the SWCC that would promote to implement our present understanding of the mechanics of unsaturated soils into conventional geotechnical and geo-environmental engineering practice applications.

In this paper, two artificial intelligent models (i.e., artificial neural networks (ANN) and multivariate adaptive regression splines (MARS)) were developed using cumulative percentiles information from GSD curve as input information to predict the SWCC of sands. The significance of each input factor from this model was critically analyzed by two different sensitivity analyses. To improve the prediction performance, a new method that combines MARS regression equation with a physicoempirical model and fitting equation using GSD curves along with basic soil properties is proposed, which is referred to as AI aid design method. The proposed novel model in this paper reliably predicts the SWCC of sandy soils.

99 MATERIALS AND METHODS

100 *Data preparation*

101 Fig. 1(a) shows grain-size distribution (GSD) data plotted as smooth curves. A typical
 102 GSD curve shown in this figure has two turning points and three segments. Seven points are
 103 highlighted on these GSD curves (i.e., P_2 , P_{50} , P_{100} , P_{250} , P_{500} , P_{1000} and P_{2000}); these points
 104 represent the cumulative percentages of particle sizes of 0.002, 0.050, 0.100, 0.250, 0.500,
 105 1.000 and 2.000 mm, respectively.

106 Following above criteria, 104 sand samples are gathered from UNSODA 2.0 database
 107 including other resources (Nemes et al. 2001, Donald (1957), Pham (2001), Lins and Schanz
 108 (2005), Likos and Jaafar (2013)). For each soil sample, information of water content and
 109 suction values from drying branches of SWCC, seven points information (i.e., P_2 , P_{50} , P_{100} ,
 110 P_{250} , P_{500} , P_{1000} and P_{2000}) from GSD curve as well as bulk density are available. A
 111 comprehensive dataset containing 1193 lines of data is generated for the 104 sand samples.
 112 Each line includes nine input parameters (i.e., seven points from the GSD curve, bulk density,
 113 and soil suction), and an output, which is the volumetric water content.

114 If some information of the particle size is missing or if it is not accessible in the database
 115 (e.g., in Fig. 1(a), the percentage value for grain size of 0.100 mm is missing), the missing
 116 value is calculated by interpolation. There are various methods for interpreting the missing data
 117 (Nemes et al. 1999). In this study, the equation below (i.e., eq. (6)) is used for gathering the
 118 information about the missing points in GSD curves.

$$119 \quad (6) \quad p_{miss} = p_0 + \frac{p_1 - p_0}{d_1 - d_0}(d - d_0)$$

120 where, p_{miss} is the missing percentile, d is the grain size at the missing point, d_0 and d_1 are the
 121 grain sizes that are available before and after the missing data, p_0 and p_1 are the accumulative
 122 percentiles at d_1 and d_2 , respectively.

123 Table 2 presents the statistical description of input and output variables. Skewness, S_k

describes asymmetry in statistical distribution; a positive value means that there is more data available that is greater than the mean value, while negative value suggests that more data is less than the average value. Kurtosis, K_u measures the data whether it is heavy- or light-tailed compared with normal distribution. The dataset with high kurtosis tends to have heavy tails, or outliers; while low kurtosis means light tails, or lack of abnormal values. These two statistical numbers are calculated based on eqs. (7) and (8).

$$(7) \quad S_k = \frac{N}{(N-1)(N-2)} \sum_{i=1}^N \left(\frac{x_i - \bar{x}}{\sigma} \right)^3$$

$$(8) \quad K_u = \frac{N(N+1)}{(N-1)(N-2)(N-3)} \sum_{i=1}^N \left(\frac{x_i - \bar{x}}{\sigma} \right)^4 - \frac{3(N-1)^2}{(N-2)(N-3)}$$

where, N is the total number of a variable, x_i is a value for an input or output variable, $\bar{x}$ is the mean value, and σ is standard variation of this variable. With above statistical information, normalization can be applied to decrease fluctuation of data (Uzielli et al. 2005). However, if the values of most data fall within a limited range (e.g., the suction is from zero to 1500 kPa), normalization is not required.

The input and output data are randomly separated into training and testing sets; 70% percentage of data form training sets and the remainder 30%, form the testing sets. The training dataset is used to train the AI models, while the testing set is used to verify the model performance.

Artificial Intelligent Models

Artificial neural networks

ANN is a widely used machine learning method that is comparable to human perception system. It is typically categorized into three layers; namely, input layer, hidden layers, and output layer, as shown in Fig. 2(a). Input layer and output layer are responsible to input and output variables, respectively. However, hidden layers contain several computation layers and

numbers of neurons. The computation results obtained for this layer are applied to next layer and are optimized by back distributing errors from output layer to each neuron in the former layer (LeCun et al. 2015).

Each input variable is randomly assigned weight, w_i and bias b when it transmits to neurons in hidden layers. There is an activation function referred to as transfer function between hidden and output layers, controls the neuron's expression (LeCun et al. 2015). One of the frequently used transfer functions is a sigmoid function, i.e., eq. (9), which is a smooth line from zero to one.

$$(9) \quad \text{sigmoid}(x_p) = \frac{1}{1 + e^{-x_p}}$$

where, x_p is the value in previous layer before output layer.

ANN has the ability of simulating the complex nonlinear relationships between input and output variables owing to its unique architectures (i.e., neurons and activation functions as shown in Fig. 2(b)). However, it behaves like a black box; due to this reason, it is difficult to judge what happens within the model. This is one of the key limitations of ANN.

Multivariate adaptive regression splines

MARS is a nonlinear regression model that mimics the knots and splines from a tree structure. Unlike traditional models (e.g., Lasso and OLS), MARS can tolerate the specification of more complex terms (Friedman 1991). It splits data into several splines using the equivalent intervals and separates each of the spline further into several subgroups by knots. The knots can be created between different input variables or various intervals at the same input.

A hinge function as shown in eqs. (10) and (11) works as a knot that separates a continuous line into two subgroups. Two or more hinge functions can be multiplied together to create new features. With these features, a basis function can be developed for each subgroup (Friedman 1991). The relationship between hinge function and basis function is plotted in Fig.

173 2(c), where a knot is separated by hinge function while a segment of line is described by a basis
 174 function.

$$175 \quad (10) \quad h(x) = \begin{cases} \max(0, x - t_k), & \text{if } x \geq t_k \\ \max(0, t_k - x), & \text{if } x < t_k \end{cases}$$

$$176 \quad (11) \quad \max(0, x - t_k) = \begin{cases} (x - t_k), & \text{if } x \geq t_k \\ 0, & \text{if } x < t_k \end{cases}$$

177 where, x is a value for an input variable, $\max()$ is a function to obtain maximum value, and t_k
 178 is a separating point. A general MARS model is expressed in eq. (12). To select the most
 179 significant terms in MARS model, a generalized cross-validation (GCV) function suggested by
 180 Friedman (1991) is used as shown in eq. (13).

$$181 \quad (12) \quad f(X) = \beta_0 + \sum_{i=1}^N \beta_i \times BF_i(X)$$

$$182 \quad (13) \quad GCV = \frac{1}{N} \sum_{i=1}^N \left(\frac{O_i - P_i}{1 - k/N} \right)^2$$

183 where, X is the input variable, β_i is constant determined by MARS, BF_i is the i th basis function,
 184 $f(X)$ is output variable and it refers to as the predicted volumetric water content in this study,
 185 O_i is the observation value (i.e., measured volumetric water content in this study), P_i is a single
 186 predicted water content value corresponding to specific soils properties (i.e., GSD and bulk
 187 density) and suction, and k is effective number of parameters; this value is calculated by MARS
 188 model based on the number of knots and GCV model parameter penalty per knot in Table 6.
 189 This value equals 33.5 for the study in this paper.

190

191 ***Model performance criteria***

192 Several statistical indices are widely used to compare prediction accuracy of AI models,
 193 including the coefficient of determination (R^2), root mean square error (RMSE) and Bias. In
 194 other words, these statistical indices (i.e., eqs. (14), (15) and (16)) can be used to evaluate the
 195 model performance.

$$R^2 = \frac{[\sum_{i=1}^N (O_i - \bar{O}_i)(P_i - \bar{P}_i)]^2}{\sum_{i=1}^N (O_i - \bar{O}_i)^2 \sum_{i=1}^N (P_i - \bar{P}_i)^2} \quad (14)$$

$$\text{RMSE} = \left[\frac{1}{N} \sum_{i=1}^N (O_i - P_i)^2 \right]^{1/2} \quad (15)$$

$$\text{Bias} = \frac{1}{N} \sum_{i=1}^N (P_i - O_i) \quad (16)$$

where, $\bar{O}_i$ and $\bar{P}_i$ are the mean values of the observed and predicted variables, respectively. If the value of R^2 is approaching one, the predicted values are close to the measured data (Moradi et al. 2019). The errors associated with prediction values will be lower when RMSE and Bias values are closer to zero.

RESULTS

Figs. 3(a) and (b) summarize the results of ANN model performance. All the parameters in the ANN model are determined by ‘trial-and-error’ method. The key model parameter is the number of hidden layers; the best value of this parameter has been estimated to be as nine using the above method. The parameters details for ANN and MARS are listed in Table 6.

The R^2 values for training and testing data sets in ANN model are 0.92 and 0.88, respectively. The data points distribution reveals that most of the predicted values fall in the range between $\pm 15\%$ of the measured values. The prediction errors from statistical indices; namely, RMSE for training part is 3.53 in comparison with 4.22 for testing results and Bias value for training is -0.02, while for testing part is -0.08. Both the statistical indices and data distribution suggest that the ANN has the ability to predict SWCC with a reasonable degree of accuracy.

Figs. 3 (c) and (d) highlight the details of the prediction performance of MARS model. The R^2 values for training and testing sets are 0.85 and 0.82, respectively; these values are slightly lower than ANN model. For the output distribution, most data locate in the range between $\pm 15\%$ of measured values. Several points are however a bit far from the line of

equality (i.e., 1:1 straight line). RMSE values both for training (4.63) and testing (5.04) data sets are higher than the corresponding values of ANN model. As for Bias index, although it is 0.0 for training data set, the value for testing data set is 0.29, which is higher than that of ANN. Statistical indices and output distribution both indicate that MARS model has weaker performance than ANN model in terms of prediction of the SWCC.

A regression equation linking input variables to output values based on basis functions is generated in MARS model as a part of the results (i.e., Table 3 and eq. (17)). In this equation, 13 basis functions are used. The coefficients before each basis function, i.e., β_i in eq. (12), is determined automatically based on the entire dataset (i.e., 104 sand samples with 1193 lines of data). It should be noted that for different datasets, the regression equation is distinct. However, the equation is less sensitive to MARS model parameters (i.e., the equation provides approximately the same results for similar model parameters). This discussion suggests that MARS approach is more stable, and hence this approach is promising for use in engineering practice applications.

$$(17) f(X) = 105.79 + 23.05 BF1 - 22.18 BF2 + 0.11 BF3 + 0.37 BF4 + 0.18 BF5 - 23.24 BF6 + 0.51 BF7 - 0.42 BF8 - 3.87 BF9 - 0.64 BF10 - 0.08 BF11 + 4.66 \times 10^{-3} BF12 + 0.77 BF13$$

where, BF is the corresponding basis function in Table 3.

Interestingly, only three input variables; namely, P_{100} , bulk density ρ_b and soil suction ψ are used to construct basis functions in the MARS model. The SWCC can be predicted with reasonable accuracy using information of only one data point from GSD curves, although regression equation is complex; with 13 basis functions and the coefficients are determined using the entire dataset.

The comparison of predicted SWCCs with measured data for several soils are plotted in Fig. 4. There is a good comparison between the predicted and measured SWCC for most sands. This model can also be used for predicting the SWCC of sands with distinct bulk density,

as shown in Figs. 4(e) and (f). However, for several sands, MARS can only predict the basic shape of SWCC but is not close to the measured SWCC (e.g., Figs. 4(a) and (d)).

Sensitivity analyses

Two groups of sensitivity analyses were conducted for examining the validity of the input parameters. In first group, one input variable is removed, and the remainder of input information is used in the model. The results are shown in Table 4 and Fig. 5 (i). In second group, two input variables are used, and one is a fixed input, which is soil suction ψ . The results of the analyses are shown in Table 5 and Fig. 5 (ii). The model name denotes the removed input variable or utilized input following the listed variable order in Table 2 (i.e., P_2 , P_{50} , P_{100} , P_{250} , P_{500} , P_{1000} , P_{2000} , ρ_b , and ψ). For example, in first group, *M9* means soil suction ψ is removed from input while other input parameters remain in the model. In second group, *U2* means that the adopted input variables are P_{50} and soil suction ψ . As discussed earlier, soil suction ψ is always used as input for each model in the second group analysis.

Fig. 5(a) shows that R^2 and RMSE values change slightly when one input variable from GSD curves (i.e., from P_2 to P_{2000}) is deleted from the ANN model. However, without soil suction (i.e., *M9*), R^2 value drops significantly and RMSE increases drastically. These results suggest that removing one of input variables from the GSD curve has little impact on the model accuracy. However, model prediction performance is highly sensitive to soil suction. MARS sensitivity analysis results summarized in Fig. 5(b) also highlight this point.

Evaluation of MARS model

MARS model facilitates in providing a rational explanation on the significance of GSD curves in the prediction of SWCC. This can be explained using Fig. 5(b) along with Table 4. From model *M1* to *M7*, it can be derived that when one input variable is deleted, neighbouring

points of GSD curves can be used to construct basis functions. For example, if P_{500} is deleted in $M5$, the adjacent data point P_{1000} can be used as an alternative to build the regression equation. However, statistical values of $M2$ and $M4$ (R^2 values are 0.84 and 0.86, respectively) in Fig. 5(b) suggest that even adopting the same input variables, the MARS models are distinct. This means that each input variable has some contribution to the MARS regression equation.

From first group of sensitivity analysis, MARS model can predict SWCC with a reasonably high degree of accuracy using a basic soil property (i.e., bulk density, ρ_b) and one point from the GSD curve (i.e., percentile at particle size 0.100 mm, namely P_{100}). This may be derived from GSD characteristics, as shown in Fig. 1(a), P_{100} that is typically close to the turning points. As MARS splits data into splines, the turning points are more easily recognized as key knots to separate data. Therefore, the point (i.e., P_{100}) can be used as a key input parameter into the MARS regression equation. The second group sensitivity analysis provides explanation on the significance of each input from the GSD curve and a basic soil property, i.e., bulk density, ρ_b .

Figs. 5 (c) and (d) highlight similar trends using two input variables both in ANN and MARS models. The R^2 values for these two models are close with small differences in their values of RMSE. These results suggest that both models have similar prediction performance using limited soil information.

Figs. 5 (c) and (d), from $U1$ to $U8$, show the significance of each input is different. It is clear with P_{100} (i.e., $U3$), both models provide high accuracy. Moreover, with neighbouring points (i.e., P_{50} in $U2$ and P_{250} in $U4$), ANN and MARS models also achieve relatively reasonable predictions, i.e., R^2 values are around 0.8. However, if only one point is used in the GSD curve, the prediction errors are high; for example, all RMSE values in $U2$, $U3$ and $U4$ are above 5.0 in ANN. Except models $U2$, $U3$ and $U4$, prediction performance for $U5$ (inputs are percentiles P_{500} and soil suction ψ) is better. R^2 value in $U5$ is around 0.80 for MARS model,

which is higher than other models. As explained earlier, this point (i.e., P_{500}) is close to the other turning point in GSD curve.

[Table 5](#) lists the total number of basis functions used to construct MARS regression expression to discuss the influence of the number of basis functions. In $U3$, 11 basis functions are required, and in $U4$, 12 basis functions were used. However, statistical indicators suggest, $U3$ provides a better prediction performance. The major difference between $U3$ and $U4$ is the selected point (i.e., P_{100} in $U3$ and P_{250} in $U4$) in GSD curve; this discussion suggests that the selected variable has significant effect on the results for MARS model.

DISCUSSION

There may be a concern when available GSD information, say for example, P_{100} is not reliable. However, these values can be inferred from GSD curves without losing accuracy using [eq. \(6\)](#). This is discussed in earlier section and the effect is highlighted in [Fig. 1\(a\)](#); it is possible to estimate the information from the typical GSD curve even if the information of several measured points is missing. Therefore, with inferred GSD points, the particle size information can be used with confidence to obtain reliable results.

[Fig. 3](#) shows that MARS model is less accurate than ANN. However, from [Fig. 5 \(ii\)](#), it can be observed that these two models will have similar accuracy, if one cumulative percentile information from the GSD curve is used as input. It means that ANN is more flexible with more inputs. This can be explained from the unique structure of ANN in [Figs. 2 \(a\)](#) and [\(b\)](#). Due to the nonlinear form activation function before output in each neuron, the contribution of each input towards output is distinct. While for MARS, as shown in [Fig. 2\(c\)](#) and [eqs. \(10\)](#), [\(11\)](#) and [\(12\)](#), the hinge function for each part of data is similar to a linear equation. Obviously, linear-form functions in MARS would generate higher prediction errors, as the dataset is more complex and nonlinear.

However, due to the larger degree of flexibility, the results highlight some fluctuations when the ANN is trained in MATLAB R2019a (The Mathworks Inc., Natick, MA, USA) as shown in Fig. 6 (i). In other words, the model performance varies with model training process for the same ANN parameter. For example, when ANN is first built (i.e., the first time in Fig. 6 (i)), R^2 is 0.88; however, when ANN has been trained six times in the platform, the R^2 value drops to 0.86. Despite achieving similar R^2 values, other statistical indicators are distinct, e.g., the RMSE values at the second and ninth times. In this paper, the results at the ninth time are adopted, where ANN achieves the best prediction performance as shown in Fig. 6 (i). The convergence curve in Fig. 6 (ii) reveals that at iteration epoch 168, ANN gains the lowest error.

Information of four soils samples were collected from Zhai et al. 2018 and Gallage and Uchimura (2010) to further evaluate MARS model prediction performance. The MARS model prediction results are plotted in Fig. 7. These results suggest that that MARS model can also predict SWCCs that do not belong to the database. The shape of SWCC can also be reasonably estimated. For example, the SWCC for fine sand and Edosaki sands in Figs. 7 (a), (c) and (d) are well predicted. In addition, some key details such as the segment near air-entry value for clayey sand are well predicted (i.e., Fig. 7(b)). However, for soils with higher fine contents, the prediction model starts losing some accuracy. Such a behavior can be attributed to the limited data of clayey SWCCs in the database. More investigation studies on model variance are conducted to explain the soil performance with distinct input values.

Fig. 8 presents two sets of model variance for a typical sand and a loamy sand, as an example. The role of bulk density is similar for these two sands. The variance of bulk density only affects the boundary effect zone and the transition zone of the SWCC. However, when suction value approaches close to zero, the variation of water content is larger. The variance of P_{100} for these two sands is distinct. For sand, when P_{100} value is increasing, the entire SWCC including the residual zone shifts upwards (i.e., the volumetric water content at different

suction values increases a similar value). It is however interesting to note, for loamy sand, the variance of P_{100} is different. Such a behavior may be attributed to the structure of MARS expression (i.e., eq. (17) and Table 3. One term, $BF10$, controls the expression of P_{100} . When P_{100} exceeds 20.1, $BF10$ will be zero and no other term makes up for this loss. Since this term is added directly to MARS expression (i.e., eq. (17)), when it is larger than 20.1, and increase of P_{100} will not shift the whole SWCC in a parallel fashion. Therefore, the SWCC prediction for clayey soil is less accurate due to higher clay content and P_{100} value.

From Fig. 5(b) and Table 4, the R^2 and RMSE values for $M3$ are respectively 0.87 and 4.37. These values suggest that $M3$ prediction performance is better in comparison to both training and testing sets of original MARS model in Figs. 3 (c) and (d). However, close observation of predictions of $M3$ suggest some abnormalities. For example, for Hostun sand in Fig. 3(f), the volumetric water content rises first and drops rapidly as suction increases in the residual zone. Although the total errors between prediction values and measured data are lower in $M3$, this model lacks physical meaning.

As shown in Fig. 5 (ii), it might be simpler and more flexible to use information (i.e. P_{100}) from the GSD curves to build prediction regression using MARS. This is because the accuracy achieved using one point or one point with bulk density (i.e., P_{50} , ρ_b and ψ) is approximately the same. From Fig. 1(a), it is noticeable that GSD curve only includes soil particle information that are divided into clay, silt, and sand from zero to 2 mm as grain size increases. However, the pore size distribution also influences the SWCC behavior (Fredlund and Rahardjo 1993, Zhou 2013, Zhai et al 2020). Therefore, it is plausible to predict SWCC using one point from the GSD curve along with bulk density.

This paper only focuses on SWCC prediction for sands because the information for clay and silt samples is limited in the database used in the present study. In addition, there are several factors that influence the SWCC behavior of fine-grained soils that include, soil texture,

plasticity index, initial water content, initial dry density, confining pressure, and temperature (Vanapalli et al. 1999, Tripathy et al. 2014, and Burton et al. 2020). However, information of these parameters is not available in the database used in the present study, for fine-grained soils. Therefore, this paper is limited to the prediction of SWCC for sands using the GSD curves and bulk density. The adaptability of AI models to other significant factors (e.g., soil fabric, Atterberg limits, initial water content, initial dry density) which predominantly contribute to the SWCC of fine-grained soils (i.e. clay and silt) needs further research.

A combined prediction method

The summarized discussions in earlier section suggest that MARS prediction is reasonable but not accurate for some soils. The MARS regression model relies more on database than providing physical explanation. There are other models in the literature referred to as physicoempirical models that are used for predicting the SWCC with the information of soil physical properties and empirical fitting parameters along with the GSD curve. For example, Arya and Paris physicoempirical model is based on dry density, void ratio, and fitting parameter α_{AP} (Arya and Paris 1981, Arya et al. 1999), which is eq. (1) (shown in Table 1). Therefore, a new prediction method combining AI features with physico-empirical model and fitting equation is proposed. As shown in Fig. 9, two steps are required for implementing this method.

The first step is to obtain the MARS regression model (i.e., eq. (17) shown in Table 3). The SWCC for the target sandy soils can be predicted using suction values, $\psi = 0.001, 0.010, 0.100, 0.491, 0.981, 1.962, 3.924, 4.905, 9.810, 19.620, 39.240, 49.050, \text{ and } 98.100$ kPa as well as P_{100} in GSD curve and bulk density as input information. The suction values are fixed from 0.001 to 98.100 kPa because this suction range is large enough to capture the key features of the SWCC for most sands for three distinct zones; namely, the boundary effect zone, transition

zone and residual zone (Vanapalli et al. 1999). These three zones typically fall within this suction range of 0 to 100 kPa or less for coarse-grained soils such as sands and some sandy soils; however, for fine-grained soils such as clay and fine-grained silts, an extended suction range is required to capture the SWCC information for the three different zones.

The calculated SWCC from MARS regression equation is then calibrated to achieve continuity from saturated condition up to the air-entry value of the soil. A calibration parameter is introduced as given below.

$$(18) \quad \theta_{vc} = S^{\kappa} \theta_c$$

where, θ_c is the calculated volumetric water content, θ_{vc} is the calibrated value, and S^{κ} is an empirical parameter. In the term S^{κ} , degree of saturation is referred to as S and κ is a fitting parameter. The parameter S^{κ} is determined by the calculated SWCC in MARS model and measured saturated volumetric water content. For example, if the measured saturated water content is 0.36, the calculated value from MARS model is 0.3, and S^{κ} equals 1.2. Usually, it ranges from 0.75 to 1.25 to ensure the predicted SWCC in MARS model is consistent with saturated condition prior to the air-entry value.

The second step is to fix the Arya and Paris model parameter α_{AP} using calibrated SWCC points discussed in the previous step. When parameter α_{AP} varies, there is minimum distance between calibrated SWCC and calculated SWCC from Arya and Paris model. The distance is expressed as sum of square of deviation (Arya et al. 1999) by eq. (19).

$$(19) \quad d_{min} = \min (\sum_{i=1}^N d_i^2)$$

where, $\min ()$ is a function to find the minimum value, d_{min} refers to as the minimum distance, and d_i is the distance for a single point in SWCC between calibrated value and calculation result using Arya and Paris model. A reliable SWCC can be obtained from Arya and Paris model by finding the suitable parameter α_{AP} from eq. (19). This is realized using calibrated SWCC values derived from MARS regression equation. The prediction performance in this stage is plotted

in Fig. 10.

Finally, Fredlund and Xing equation (Fredlund and Xing 1994) (i.e., eq. (20)) is applied to the predicted results to obtain a smooth-form SWCC. This is realized by finding a set of fitting parameters (i.e., a_f , m_f , and n_f) through a least-squares method (i.e., eq. (21)).

$$(20) \quad \theta_{FX}(\psi, a_f, m_f, n_f) = \left\{ 1 - \frac{\ln(1 + \psi/\psi_r)}{\ln[1 + (1000000/\psi_r)]} \right\} \frac{\theta_s}{\{\ln[e + (\psi/a_f)^{n_f}]^{m_f}\}}$$

$$(21) \quad T(a_f, m_f, n_f) = \min(\sum_{i=1}^N (\theta_{AP} - \theta_{FX})^2)$$

where, ψ_r is residual suction, θ_s is saturated volumetric water content, e is base of natural logarithm, a_f , m_f and n_f are fitting parameters, θ_{AP} is the predicted volumetric water content from Arya and Paris model, θ_{FX} is the calculated volumetric water content from eq. (20), and compare with $T(a_f, m_f, n_f)$, which is the objective function (i.e., eq. (21)).

In this method, only basic soil properties (i.e., saturated volumetric water content, bulk density and particle density for Arya and Paris model, as well as GSD curves) are required for calculation purpose. In addition, the only parameter S^* is set to achieve continuity of the SWCC starting with initially saturated condition. For convenience, this method is referred to as AI aid design method in order to distinguish from traditional fitting method, for which the model parameters are determined mainly from SWCC that is measured in the laboratory or from field tests.

For this method, AI model (i.e., MARS regression model) is used for obtaining an approximate SWCC. However, physico-empirical model (i.e., Arya and Paris model) along with the MARS regression method, which is referred to as the AI aid design method is useful in the prediction of reliable data for SWCC. The fitting equation (i.e., Fredlund and Xing equation) facilitates in obtaining a best-fit SWCC from Arya and Paris model. Each model (e.g., MARS) can independently generate SWCC; however, these models have certain limitations. Therefore, we combined them together to alleviate the limitations and predict a

continuous SWCC with a reasonably high accuracy using only the information of grain size distribution. All these models are performed in MATLAB R2019a, which can easily visualize the results in each step.

In this study, only drying branches of SWCC are discussed. It is well known that several factors contribute to the SWCC hysteresis behavior such as the contact angle, entrapped air, and water retention capacity of soil pores during drying-wetting cycles (Fredlund and Rahardjo 1993). However, hysteresis behaviors of the SWCCs are complex (Zhou 2013) and modelling this process by AI methods (e.g., AI models and AI aid design method) needs further research.

The performance from the AI aid design method is plotted in Fig. 11. The predicted curves are plotted as continuous black curves. The prediction results for various sands both from the database and sample data in the literature are compared. From Fig. 11, the predicted SWCC by the AI aid design method is close to the measured SWCC data (i.e., solid orange dots). Comparing with MARS results (i.e., triangles) in Fig. 10, the prediction performance using AI aid design method is reliable in predicting the all the key features of SWCC for various sands in the different zones (i.e., boundary effect, transition, and residual zones).

CONCLUSIONS

In this paper, ANN and MARS models are proposed for rapid prediction of the SWCC using GSD curve and bulk density. The ANN is found to be reasonably accurate and flexible due to the use of activation function before output layer. However, MARS is a more stable model because it implements a regression equation with several basis functions. Reasonable prediction of the SWCC is possible for both models using one point (i.e., P_{100}) in GSD curve and bulk density along with soil suction.

Through two distinct sensitivity analysis, P_{100} in GSD curve was established as the key input variable; it is also possible to predict SWCC simply from one point i.e., P_{100} in GSD

curve and soil suction information.

A more rigorous method (i.e. AI aid design method) is developed by combining MARS along with Arya and Paris model and Fredlund and Xing equation. This two-step method only requires basic soil properties that include saturated volumetric water content, bulk density, particle density and GSD curves. One calibration parameter S^* , which typically ranges from 0.75 to 1.25, is introduced for achieving a continuous SWCC that starts from fully saturation condition. The proposed method rapidly and reliably predicts the SWCC of sands.

ACKNOWLEDGEMENT

The first author gratefully acknowledges and appreciates the China Scholarship Council and University of Ottawa, Canada for joint funding his Ph.D. research program. The second author thanks the support from NSERC for his research programs. The first author would like to thank Dr. Hossein Bonakdari, who offered the AI course, which helped in learning fundamental concepts of AI. The authors sincerely thank the constructive criticism of the reviewers that has significantly contributed to improve this paper.

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FIG. 1. Typical GSD and SWCC curves for loamy sand (UNSODA 2.0, Soil No. 1011).

FIG. 2. Illustration of ANN model and relationships of MARS functions.

FIG. 3. Prediction performance of ANN and MARS models.

FIG. 4. Comparison of predicted SWCC with measured data based on MARS model.

FIG. 5. Two groups sensitivity analyses for ANN and MARS models.

FIG. 6. Running fluctuations and computation convergence of ANN model.

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FIG. 10. Prediction performance from Arya and Paris model based on calibrated MARS results.

FIG. 11. Prediction results using proposed AI aid design method.

(a) Grain size distribution curve

(b) Soil-water characteristic curve

(The air-entry value and residual suction are predicted based on [Vanapalli et al.1998](#))

FIG. 1. Typical GSD and SWCC curves for loamy sand (UNSODA 2.0, Soil No. 1011).

FIG. 2. Illustration of ANN model and relationships of MARS functions.

FIG. 3. Prediction performance of ANN and MARS models.

Note: Blue triangles are the measured data from the dataset while red continuous curves are predicted values.

FIG. 4. Comparison of predicted SWCC with measured data based on MARS model.

FIG. 5. Two groups sensitivity analyses for ANN and MARS models.

Part (i) Running fluctuations of ANN model

Part (ii) Computation convergence of adopted ANN model

Note: In Part (i), bar graph shows R^2 values, red line denotes RMSE values while blue line represents Bias values. In Part (ii), the black line shows the epoch with lowest error.

FIG. 6. Running fluctuations and computation convergence of ANN model.

Note: Blue points are experimental data while red curves are prediction values. Data is collected from [Gallage and Uchimura \(2010\)](#) and [Zhai et al. 2018](#).

FIG. 7. MARS model prediction performance using the data outside the database.

Notes: The cyan dots are the measured data. The blue line with dots is the predicted SWCC with initial P_{100} and bulk density.

FIG. 8. Variance of MARS model input variables.

FIG. 9. Overall framework of proposed AI aid design method for SWCC prediction from GSD curves and basic soil properties.

Note: Orange circles are measured data, green triangles are MARS performance, and the black lines are curves predicted by Arya and Paris model based on calibrated MARS results.

FIG. 10. Prediction performance from Arya and Paris model based on calibrated MARS results.

Note: Solid orange circles are measured data, black open circles are data derived from AI aid design method and continuous black lines are best-fit curves using Fredlund and Xing (1994) equation.

FIG. 11. Prediction results using proposed AI aid design method.

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Table 1. Models for predicting the SWCC from the GSD curve.

Eq. # and References	Equations and Notations
Eq. (1) Arya and Paris (1981) and Arya et al. (1999)	$\begin{cases} \theta_{vi} = S_f \sum_{j=1}^i \rho_b (W_i / \rho_P) e \\ \psi_i = 2T_s \cos \theta / [\rho_w g R_i \{2e [3W_i / (4\rho_P \pi R_i^3)]^{1-\alpha_{AP}} / 3\}^{1/2}] \end{cases}$ <p>where, θ_{vi} is the average volumetric water content represented by pore volume that corresponds to ith particle size range, S_f is scale factor and defined as the ratio of theoretical volumetric water content to porosity, ρ_b is bulk density, W_i is solid mass per unit mass in the ith particle size range, ρ_P is particle density, e is void ratio, ψ_i is soil suction, T_s is surface tension, θ is contact angle, ρ_w is water density, g is acceleration of gravity, R_i is the mean particle size in ith grain size range, and α_{AP} is fitting parameter.</p>
Eq. (2) Tyler and Wheatcraft (1989)	$\psi_i = 2T_s \cos \theta / [\rho_w g R_i (2e N_i^{1-D} / 3)^{1/2}]$ <p>where, N_i is the number of particles with radius R_i, and D is fractal dimension.</p>
Eq. (3) Fredlund et al. (2002)	$p(\phi) = p_1 \left[\frac{1}{\ln \{ \exp(1) + \left[\frac{10^{-\log(d_e) - 1}}{p_2} \right]^{p_3} \}} \right]^{p_4} + p_5$ <p>where, p_1, p_2, p_3, p_4 and p_5 are fitting parameters, d_e is effective particle diameter, and $p(\phi)$ is the value for either m_f or n_f in Fredlund and Xing (1994) model.</p>
Eq. (4) Chin et al. (2010)	$a_f = -2.4x + 722; n_f = 0.07x^{0.4}; m_f = 0.015x^{0.7};$ $\psi_r = 914 \exp(-0.002x); x = eP_{200}$ <p>where, a_f, n_f and m_f are fitting parameters in Fredlund and Xing (1994) equation, ψ_r is residual suction, and x is combination of void ratio e and percentage at soil passing standard sieve No. 200, P_{200}.</p>
Eq. (5) Zhai et al. (2020)	$A_{void}^{Total} = \sum_{i=1}^N P_i P_j P_k (s_{tri} - 0.5\alpha_t r_k^2 - 0.5\beta_t r_i^2 - 0.5\gamma_t r_j^2);$ $r_{tangen} = \frac{1}{r_i} + \frac{1}{r_j} + \frac{1}{r_k} + 2\sqrt{\frac{1}{r_i r_j} + \frac{1}{r_j r_k} + \frac{1}{r_k r_i}};$ $\psi = 2T_s \cos \theta / (\rho_w g r_{tangen}); S = \frac{A^m}{A_{void}^{Total}}$ <p>where, A_{void}^{Total} is total void area, P_i, P_j and P_k are the probabilities filling the triangle between particles with radii of r_i, r_j and r_k, s_{tri} is the area of triangle, α_t, β_t and γ_t are three angles of the triangle, r_{tangen} is the circle that is tangent to all three particles, ψ is soil suction, S is degree of saturation, and A^m is the total area filled with water.</p>

Table 2. Statistical description of input and output variables.**

Variable	Minimum	Average	Maximum	Skewness	Kurtosis
P_2 (%)	0.00	3.74	10.40	0.56	0.15
P_{50} (%)	0.09	10.58	20.46	0.48	-0.36
P_{100} (%)	0.70	21.34	52.81	0.48	-0.38
P_{250} (%)	6.50	59.17	100.00	-0.57	-1.01
P_{500} (%)	20.00	82.90	100.00	-1.41	0.74
P_{1000} (%)	70.30	96.40	101.70	-2.33	5.00
P_{2000} (%)	91.00	99.86	102.30	-6.25	46.37
ρ_b (g·cm ⁻³)	1.27	1.56	1.80	-0.19	0.15
ψ (kPa)	0.00	56.68	1617.67	6.01	35.29
θ^{**} (%)	0.00	19.39	51.70	0.39	-1.10

Notes: ρ_b is bulk density, ψ is soil suction, and θ is volumetric water content.

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Table 3. Basis functions for MARS prediction model.

BF No.	Expression	BF No.	Expression
<i>BF1</i>	$\max(0, x_9 - 8.72)$	<i>BF2</i>	$\max(0, 8.72 - x_9)$
<i>BF3</i>	$BF2 \cdot \max(0, x_3 - 3.07)$	<i>BF4</i>	$BF2 \cdot \max(0, 3.07 - x_3)$
<i>BF5</i>	$\max(0, x_9 - 27.47)$	<i>BF6</i>	$\max(0, x_9 - 4.91)$
<i>BF7</i>	$\max(0, 4.91 - x_9) \cdot$ $\max(0, x_3 - 9.8)$	<i>BF8</i>	$\max(0, 4.91 - x_9) \cdot$ $\max(0, 9.8 - x_3)$
<i>BF9</i>	$BF2 \cdot \max(0, x_8 - 1.32)$	<i>BF10</i>	$\max(0, 20.1 - x_3)$
<i>BF11</i>	$\max(0, 27.47 - x_9) \cdot$ $\max(0, x_3 - 45.87)$	<i>BF12</i>	$\max(0, 27.47 - x_9) \cdot$ $\max(0, 45.87 - x_3)$
<i>BF13</i>	$\max(0, 45.87 - x_3) \cdot \max(0, 4.91 - x_9)$		

Notes: BF No. refers to the number of each basis function, x_3 refers to P_{100} , x_8 is the bulk density, and x_9 is soil suction ψ .

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Table 4. Variable information in first group sensitivity analysis for MARS.

Model	Omitted Variable	Utilized Variable	Model	Omitted Variable	Utilized Variable
<i>M1</i>	P_2	P_{100}, ρ_b, ψ	<i>M2</i>	P_{50}	P_{100}, ρ_b, ψ
<i>M3</i>	P_{100}	$P_{50}, P_{500}, \rho_b, \psi$	<i>M4</i>	P_{250}	P_{100}, ρ_b, ψ
<i>M5</i>	P_{500}	$P_{100}, P_{1000}, \rho_b, \psi$	<i>M6</i>	P_{1000}	P_{100}, ρ_b, ψ
<i>M7</i>	P_{2000}	$P_{100}, P_{1000}, \rho_b, \psi$	<i>M8</i>	ρ_b	P_{100}, P_{1000}, ψ
<i>M9</i>	ψ	P_{100}			

Notes: Omitted variable is the removed variable from input information; Utilized variables are the variables used to build basis functions.

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Table 5. Input variables and basis functions for MARS in second group sensitivity analysis.

Model	Input Var.	No. BF	Model	Input Var.	No. BF
<i>U1</i>	P_2, ψ	7	<i>U2</i>	P_{50}, ψ	12
<i>U3</i>	P_{100}, ψ	11	<i>U4</i>	P_{250}, ψ	12
<i>U5</i>	P_{500}, ψ	14	<i>U6</i>	P_{1000}, ψ	12
<i>U7</i>	P_{2000}, ψ	7	<i>U8</i>	ρ_b, ψ	10

Notes: Input variable is the variable used as input in MARS; No. BF is the total number of basis functions in MARS regression model.

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Table 6. Parameters of ANN and MARS models.

ANN parameter	Value	ANN parameter	Value
Number of hidden layers	9	Number of neurons in each layer	9
Training function	Levenberg-Marquardt backpropagation	Performance function	Mean square error
Transfer function	Sigmoid	Iterations number	5000
MARS parameter	Value	MARS parameter	Value
GCV penalty per knot	3	New variable penalty	0.1
Maximum Iterations	5000	Stop threshold	10^{-5}
Model prune	True	Input self-iterations	False