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Artificial neural network prediction of the water retention curve from physical soil parameters: comparing continuous and pointwise approaches

Prédiction par un réseau de neurones artificiels de la courbe de rétention à partir des paramètres physiques du sol : comparaison des approches continue et par points

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ABSTRACT: The soil water retention curve (SWRC) is a key characteristic for solving unsaturated transient hydraulic and coupled hydromechanical problems in geotechnical applications. Its determination in the laboratory is however still costly, time-consuming, and uncertain. Several pedo-transfer functions able to predict the SWRC based on the soil physical properties were developed but their applicability is generally restricted by the limited locally or regionally available soils data. With the recent developments, the availability of large international databases and the bringing into the practice of machine and deep learning algorithms, allowed the elaboration statistics-empowered predictive functions for the SWRC with improved performance. In this paper, two Artificial Neural Networks are trained to predict the curve using data extracted from the UNSODA database (Leij et al. 1996). The original dataset includes drying and wetting tests' data covering over 790 different soils from all over the world. The prediction of fitted van Genuchten (1980) model's parameters (continuous) is compared with a pointwise prediction network for which the soil suction is added to the predictors. The results show a better performance of pointwise prediction when comparing the global metrics but an advantage in the favor of the continuous prediction in terms of curve consistency.

RÉSUMÉ : La courbe de rétention de l'humidité du sol (CRHS) est une caractéristique clé dans la résolution des problèmes géotechniques dans le domaine non saturé (hydrauliques ou hydromécaniques). Sa détermination est cependant encore couteuse, longue et incertaine. Plusieurs fonctions de pédo-transfert afin de la prédire en se servant de paramètres physiques du sol mais leur applicabilité est restreinte par la représentativité locale ou régionale des données ayant servi à leur détermination. Récemment, la disponibilité de larges bases de données et la mise en pratique des algorithmes d'apprentissage automatique et profond, ont permis de proposer des fonctions prédictives plus performantes et basées sur les statistiques. Dans cette communication, deux réseaux de neurones artificiels ont été entraînés pour prédire la CRHS en utilisant des données extraites de la base de données UNSODA (Leij et al. 1996) représentant plus de 790 sols. La prédiction des paramètres du modèle continu de van Genuchten (1980) est comparée avec une prédiction point par point qui considère la succion comme un prédicteur additionnel. Les résultats montrent une meilleure performance de la prédiction point par point pour les indicateurs globaux mais donnent un avantage à la prédiction continue en termes de consistance de la courbe prédite.

KEYWORDS: Artificial neural network, water retention, machine learning, prediction, unsaturated soils.

1 INTRODUCTION

The soil water retention curve (SWRC) refers to the function describing the evolution of the soil's volumetric water content (alternatively degree of saturation) vs. suction (or pore-water potential). This function is of primary importance in various geotechnical engineering problems involving unsaturated soils. Its determination from laboratory or field hydraulic tests is however still costly and often tricky requiring the combination of different suction measurement or imposing techniques to cover the entire suction range. The highly non-linear shape of this function has led to the development of multi-parameter mathematical models to complete the description of the SWRC for the numerical modelling requirements. The high relative errors associated with suction measurement/imposition, the overlapping of techniques with varying accuracy, and the limited number of experimental points, frequently complicate the optimization process of the models' parameters. An additional complexity rises from the non-univocity of the SWRC depending on the followed path (wetting or drying).

Many researchers (Rawls *et al*. 1982, Schaap *et al*. 2001, Nemes *et al*. 2006, Baker 2008, Ghanbarian-Alavijeh & Millán 2010, etc.) had developed alternative mathematical relations to predict either the SWRC models' parameters, or pointwise SWRC based on physical and geotechnical routine identification tests as the soil bulk/dry densities, consistency limits for fine-textured soils, and the parameters of the particle-size distribution as clay/silt/sand percentages. These so-called Pedo-Transfer Functions (PTFs) are formulated using various statistical regression techniques, and more recently Artificial Neural Networks (ANNs). They are convenient in practice, but their use is often limited by the soils range covered by the dataset on which they were calibrated.

An Artificial Neural Network (ANN) is a computational method based on the simplified functioning of biological neural cells. The network is an assembly of an input layer, one or more hidden layers, and an output layer of artificial neurons. Each artificial cell, receives several input parameters, computes a weighed linear combination (with weights and bias terms), and generates an output using an activation function. The output is transmitted as an input to the next neuron until reaching the network output layer. The weights and bias terms of all cells are gradually optimized by scanning the training dataset and using the algorithm of back-propagation of error gradient, this step is referred to as the training phase. ANNs have been shown to be a very efficient technique for classification, clustering and regression tasks in different engineering and science fields. They are at the heart of Artificial Intelligence (AI) developments.

Recently, advances in using AI-based methods stimulated their application to the SWRC prediction from routine geotechnical identification parameters (essentially dry/bulk density and grain-size fractions). Large datasets issued from international databases have been used for training and testing the developed models. The SWRC is predicted using statistics-based regression algorithms with the selected most significant predictors available in the training dataset. Pham *et al*. (2019) thoroughly analysed ANN-based PTFs for SWRC prediction. Indeed, they compared different network architectures and various training algorithms and concluded that the Bayesian Regulation method outperformed the Levenberg-Marquardt and Conjugate Gradient Descent methods whatever the used architecture. Bayesian Regulation is a probability-based optimization algorithm offering the advantage of not requiring a validation subset of data as do other training methods, but its computational cost is slightly higher. Moreover, they compared using the full available dataset and a processed dataset from which outliers have been withdrawn. The ANNs trained using the processed dataset showed enhanced performance compared to the ANNs trained on the full dataset. The authors concluded that the data quality significantly influences the obtained results. Typically, two different approaches have been notably used: continuous and pointwise predictions.

The continuous approach assumes that the SWRC can be described using a mathematical equation selected among the various ones available in the literature, the van Genuchten (1980) equation being the most popular function (designated here by vG). The developed model is then designed to predict the equation's parameters using several selected input parameters. The continuous approach's main advantages are its suitability for incorporation in available numerical simulation codes and guarantee of curve shape consistency. Their drawbacks are (i) the lack of flexibility to adapt to SWRC non-standard shapes (bi- or multimodal) and to non-monotonous paths (including alternation of drying and wetting steps) and (ii) the incorporation of additional errors relative to model adequacy and to the parameters' fitting procedure.

The pointwise approach is on the contrary suited for adapting to the effective soil behavior and is theoretically able to integrate the hysteretic wetting-drying alternate paths. Nevertheless, when it is based on machine learning methods which are subject to the well-known issue of overfitting, a particular attention should be put on checking their capacity to generalize to unseen data patterns which lie out of the ranges covered by the training dataset. In the pointwise approach, the suction is used as an additional input to predict the corresponding volumetric water content resulting in a SWRC point prediction. Pros and cons, literature

This paper aims at comparing the performance of the two approaches using a SWRC dataset extracted from the UNSODA unsaturated soil hydraulic database (Leij *et al*. 1996).

2 MATERIALS AND METHODS

UNSODA contains data from 790 different soils including point records of the SWRC and hydraulic conductivity/diffusivity along with basic identification parameters as grain-size distribution data, particle density, porosity, saturated volumetric water content, *etc*.) whenever available. Abdallah (2019) by testing different machine learning algorithms concluded that the quality of data corresponding to the wetting path in UNSODA is neither quantitatively, nor qualitatively, sufficient for predicting the SWRC. Only the data issued from laboratory water retention drying tests are considered in this study. The data were mainly obtained from pressure plate and tensiometer measurements. These methods cover different ranges and have different accuracies which leads to relatively high variance in the data. As per soil classification, sands are over-represented in the database (Leij *et al*. 1996).

2.1 *Data preparation*

Based on the correlation coefficients between the candidate parameters and the target (volumetric water content), five predictors were selected (Abdallah 2019): suction, porosity, and clay/silt/sand fractions. The originally extracted dataset had to be reorganized to make it convenient for the regression analysis. For instance, redundant points, rows missing the main predictor (suction), soils with more than 50% missing data were deleted. The cleaned dataset resulted in 1551 records corresponding to 203 different soils. To avoid any effect of the variables' different magnitude, the dataset was normalized by applying the minmax scaling.

2.2 *Network architecture and training*

In this study, a standard ANN architecture in Matlab® was used. It consists of a one 10-neuron hidden layer with hyperbolic tangent (*tanh*) activation functions for all nodes. The network is trained by the Bayesian Regulation algorithm (Mathworks 2020), using a random partition of the data to 80% for training, 20% for testing.

2.3 *Pointwise SWRC prediction*

To improve the dataset quality, soils with more than 50% records containing missing parameters were deleted. The cleaned dataset is composed of 1159 records corresponding to 144 different soils. Figure 1 shows a simplified flowchart of the pointwise prediction model.

2.4 *Continuous SWRC prediction*

For each soil in the dataset, the vG model (equation 1) parameters α and n, were fitted to the suction-volumetric water content data using the Levenberg-Marquardt algorithm (Mathworks 2020).

$$\theta = \theta_r + (\theta_s - \theta_r)\left(\frac{1}{1+(\alpha\, s)^n}\right)^{\frac{n-1}{n}} \tag{1}$$

with s, being the suction while θ_s and θ_r, are the saturated and residual volumetric water content values, respectively.

When missing, θ_s was assumed equal to the porosity and θ_r was fixed to 0.1. Lower/upper bounds: $0.03 \leq \alpha \leq 5$ kPa^{-1}, and $1 \leq n \leq 5$, were imposed to keep the physical meaning of the optimized parameters based on literature (Carsel & Parrish 1988). Fittings resulting in a coefficient of determination R^2 lower than 0.75 were rejected. This process ended up with 103 records of fitted curves. Six predictors (porosity, clay/silt/sand fractions, θ_s, and θ_r) and two targets (α and n) were selected for the regression.

Different configurations have been tested for the ANN architecture and the best performance was obtained when two connected networks were used. The first standard network was used to predict n using the six predictors. The second standard network used the six predictors plus the previously predicted n, to predict α. Figure 2 shows the simplified flowchart of the prediction vG continuous model.

3 RESULTS AND DISCUSSION

In this section, the overall regression performance of the two models is evaluated on the entire dataset through the coefficient of correlation (R) and the Root Mean Standard Errors ($RMSE$) as metrics. Afterwards, the predicted SWRC on three selected reference soils are compared and discussed.

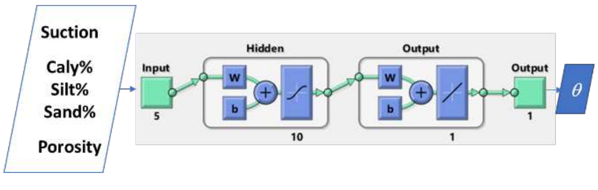

Figure 1. Flowchart of the ANN pointwise prediction model.

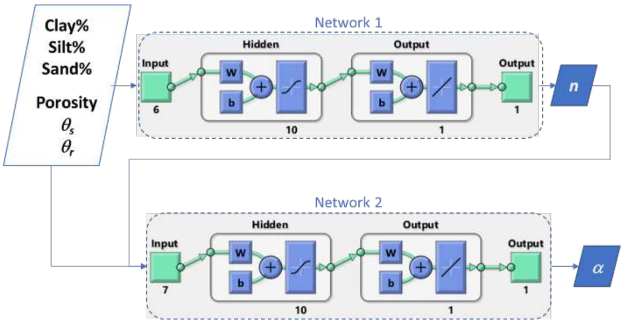

Figure 2. Flowchart of the ANN vG continuous prediction model.

3.1 *Pointwise SWRC prediction*

The predicted θ is plotted against the target value on figure 3. With a *RMSE* of 0.027, the performance of the pointwise prediction model is globally satisfactory. It is worth noticing however that the residual prediction error appears to be too high for certain points (up to 0.14). Higher residual errors concentrate around 0.35 target value which corresponds to the median θ_s value in the dataset. It is well known that suction measurement accuracy is lower for near-saturation states and this could explain this observation.

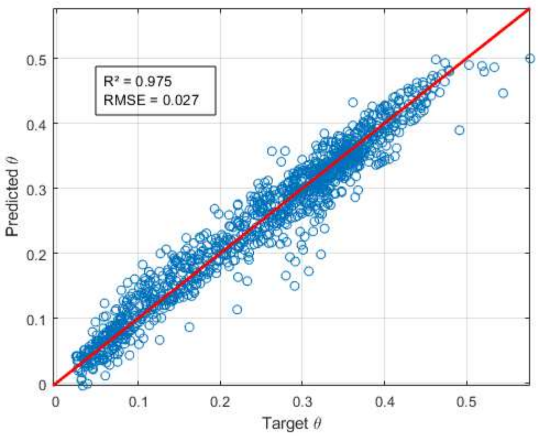

Figure 3. ANN point-wise predicted values of soil volumetric water content *vs*. measured values in the UNSODA drying laboratory tests cleaned dataset.

3.2 *Continuous SWRC prediction*

Figure 4 compares the predicted and target values of the vG parameter *n*. The overall performance of the model appears to be poor with a *RMSE* of 0.326 as compared to the median value of *n* in the dataset (1.38). This likely results from the combination of the data error with additional errors relative to the vG model adequacy and the fitting procedure.

Figure 5 shows the predicted and target values of the vG parameter α. The global performance of the model with a *RMSE* of 0.458 is quite acceptable if one omits the data points with the target value of 5 which is the upper bound imposed in the fitting procedure. A major part of the error for these points can probably be attributed to the fitting over the SWRC data series. The vG model was likely inconvenient to correctly fit the data for the corresponding soils.

3.3 *Discussion*

To further discuss the obtained results and comparatively evaluate the two approaches' performance, three reference soils (Table 1) were selected in the dataset. These soils represent at most to the maximum clay, silt, and sand contents, respectively. The position of these soils with respect to all the soils in the cleaned dataset are shown on the ternary textural diagram (Figure 6). Table 1 summarizes the main parameters of the reference soils. Given that the dataset is mainly dominated by sandy soils, the regression performance on the reference sand is expected to be better than on the references clay and reference silt.

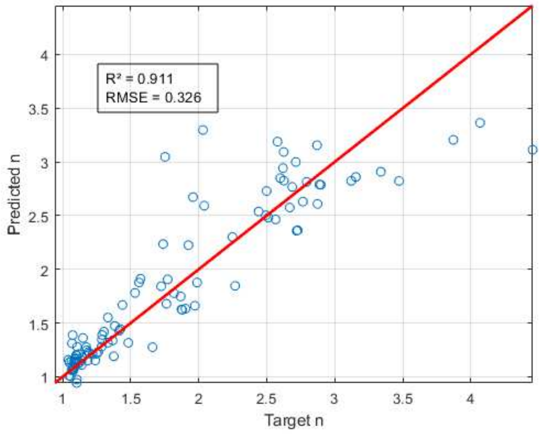

Figure 4. Continuous ANN predicted values of the *n* vG parameter *vs*. fitted values on soils' data from the UNSODA drying laboratory tests cleaned dataset.

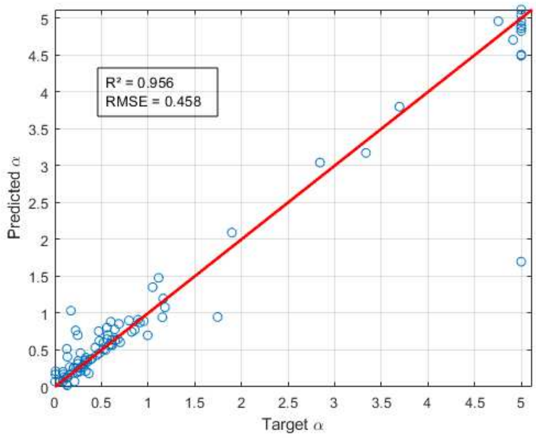

Figure 5. Continuous ANN predicted values of the α vG parameter *vs*. fitted values on soils' data from the UNSODA drying laboratory tests cleaned dataset.

Table 1. Reference soils parameters.

Reference soil	*Clay*	*Silt*	*Sand*
Sand fraction (%)	33	32	97.3
Silt fraction (%)	13	46	0 2
Clay fraction (%)	54	22	2.5
Porosity (-)	0.58	0.356	0.361
θ_s **(-)**	0.577	0.356*	0.361
θ_r **(-)**	0.1*	0.1*	0.024

**fixed to the lower or upper bound.*

Figures 7 to 9 compare the measured SWRC data with the pointwise predictions (markers) and the vG fit on measured data with the vG continuous predictions for the reference clay, silt, and sand respectively (lines). The main outcome is that the two models captured the shape of the SWRCs and successfully reproduced the range of θ. For the reference clay and silt, pointwise prediction tended to overestimate θ while the vG continuous predictions were likely to underestimate it. These trends are more pronounced on the reference clay than the on the reference silt.

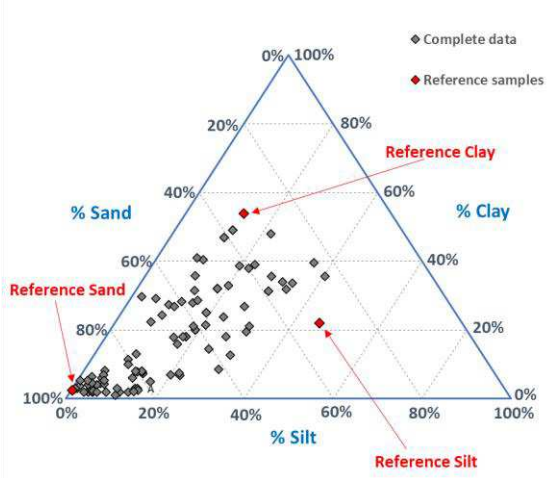

Figure 6. USCS-SCS ternary diagram for textural classification of the UNSODA drying laboratory tests cleaned dataset (represented using Graham & Midgley 2000).

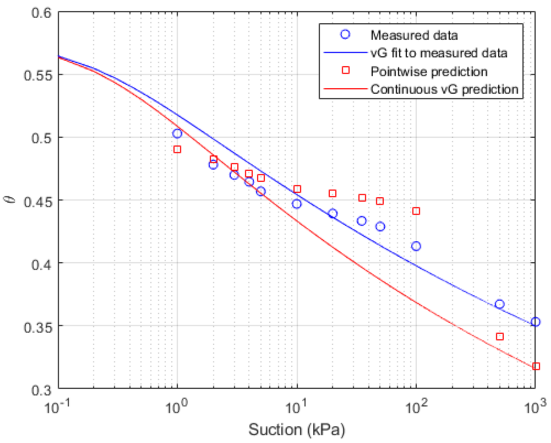

Figure 7. Comparison of the measured and fitted SWRC with the pointwise and continuous vG predicted SWRC for reference clay.

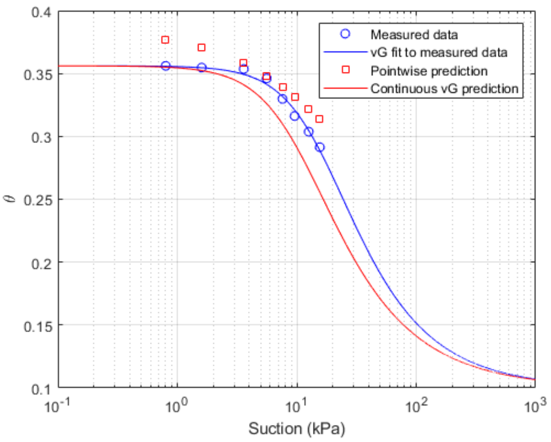

Figure 8. Comparison of the measured and fitted SWRC with the pointwise and continuous vG predicted SWRC for reference silt.

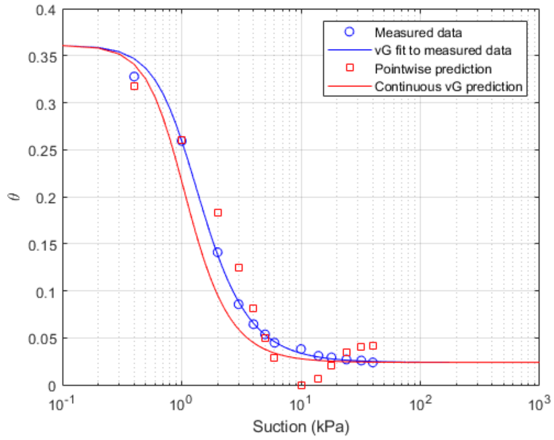

Figure 9. Comparison of the measured and fitted SWRC with the pointwise and continuous vG predicted SWRC for reference sand.

Clay soils being under-represented in the training data, the accuracy and consistence of the predictions are low as it could expected. On the reference sand, the models' predictions are quite comparable. However, even if the data is dominated by sands, the SWRC predicted by the pointwise model for the reference sand exhibits a local discrepancy around 10 kPa of suction. This kind of error is avoided when using a continuous function prediction ensuring the consistency of the predicted curve.

The use of the vG theoretical equation is shown to efficiently accommodate data imprecision. Considering the general appreciations on the entire curve's representation, the pointwise approach although having demonstrated acceptable performance, appears to be subject to local inconsistency. The use of the continuous prediction based on a mathematical model can address this issue by guaranteeing the SWRC shape theoretical compliance.

4 CONCLUSIONS

In this paper, two different approaches were used and compared for predicting the SWRC from basic geotechnical parameters. The Dataset used for training the two models was extracted from the UNSODA database and includes drying laboratory test data. The two models used feedforward ANNs trained using Bayesian Regulation algorithm. The first model (pointwise) used geotechnical parameters and suction to predict the volumetric water content providing one point of the SWRC at a time. The second model (continuous vG) used two connected ANNs to predict α and n vG parameters from geotechnical inputs.

The preliminary analysis and cleansing on the original data lead to drastically decrease the size of the dataset to favor the data quality.

Considering the standard metrics for evaluation the prediction performance on the training-testing data (*i.e., R* and *RMSE*), the pointwise prediction outperformed the continuous vG prediction. This can be attributed to the difference in the size of the datasets and to the additional errors introduced by the fitting of the vG model on experimental data series of each soil in the database.

However, after analyzing and comparing the predicted curves by the two models with the corresponding original inputs, it appeared that the continuous vG approach provided more consistent results even for all reference soils selected in the database.

Further investigations are required for improving the developed continuous vG model. Improvements could include:

- the use of alternative SWRC equations and selection of the model based on the best fit;

- investigation of using the data fitting evaluation (R^2) as an indicator for modulating the weight of the records according to the associated confidence level.

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