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# Using neural networks to predict soil water retention and soil hydraulic conductivity

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**Abstract**

Direct measurement of hydraulic properties is time consuming, costly, and sometimes unreliable because of soil heterogeneity and experimental errors. Instead, hydraulic properties can be estimated from surrogate data such as soil texture and bulk density with pedotransfer functions (PTFs). This paper describes neural network PTFs to predict soil water retention, saturated and unsaturated hydraulic properties from limited or more extended sets of soil properties. Accuracy of prediction generally increased if more input data are used but there was always a considerable difference between predictions and measurements. The neural networks were combined with the bootstrap method to generate uncertainty estimates of the predicted hydraulic properties. © 1998 Elsevier Science B.V. All rights reserved.

*Keywords:* Pedotransfer function; Neural networks; Water retention; Hydraulic conductivity

## 1. Introduction

Concern about the quality of soil and water resources has motivated the development of increasingly sophisticated models to describe water flow and solute transport in unsaturated soils. These models are generally based on numerical solutions of the Richards equation which rely on expressions for soil water retention and unsaturated hydraulic conductivity. A popular four-parameter expression for water retention is given by van Genuchten (1980):

$$S_e = [1 + (\alpha h)^{\beta}]^{1/\beta - 1} \quad (1)$$

where $h$ is the soil water pressure head; $\alpha$ and $\beta$ are curve shape parameters. $S_e$ is the relative saturation which is expressed in actual, residual and saturated volumetric water content ($\theta$, $\theta_r$, $\theta_s$) as:

$$S_e = \frac{(\theta - \theta_r)}{(\theta_s - \theta_r)} \quad (2)$$

Combination of Eq. (1) with the pore size distribution model of Mualem (1976) leads to an expression for the unsaturated hydraulic conductivity (van Genuchten, 1980):

$$K(S_e) = K_s S_e^{\delta}\{1 - [1 - S_e^{\beta/(\beta-1)}]^{1-1/\beta}\}^2 \quad (3)$$

$K$ is the hydraulic conductivity and $\delta$ is an empirical parameter that is normally fixed to 0.5 (Mualem, 1976); Schaap and Leij (1998) found that $\delta = -1.0$ was more realistic. $K_s$ is the saturated hydraulic

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conductivity and the only free parameter if $S_e$ and $\beta$ are derived from water retention measurements. Unsaturated hydraulic conductivity can also be described by the empirical expression of Gardner (1958):

$$K(h) = \frac{K_s}{1 + (ah)^b} \quad (4)$$

where $K_s$, $a$ and $b$ are the three model parameters.

Direct measurements of $\theta(h)$ and especially $K(h)$ relationships are not easily performed and in many cases not available. As an alternative, pedotransfer functions (PTFs) can be used to predict hydraulic properties from texture and bulk density. A variety of PTFs have been established with different mathematical concepts, predicted properties and input data requirements. Most PTFs are empirical and often use simple linear multiple regression equations (Gupta and Larson, 1979; Rawls et al., 1982; Vereecken et al., 1989, 1990).

PTFs can also be constructed with artificial neural networks. Studies by Pachepsky et al. (1996); Schaap and Bouten (1996); Schaap et al. (1998) and Tamari et al. (1996) show that results are often better than more traditional methods. Neural networks are sometimes described as universal function approximators which can 'learn' to approximate any continuous nonlinear function (Haykin, 1994). An advantage of neural networks, as compared to traditional PTFs, is that they require no a-priori concept of the relations between input data and output data. During an iterative calibration procedure the optimal relations between input and output data are found and implemented automatically. A drawback is that these relations are difficult to interpret because of the black-box nature of neural networks.

Several studies have reported on the use of different levels of input data to predict soil hydraulic properties (Rawls et al., 1982; Schaap and Bouten, 1996; Vereecken et al., 1989, 1990). Especially the addition of one or two water retention points to soil textural data improved the predictability of water retention and $K_s$ (Rawls et al., 1982; Ahuja, 1989 and Schaap et al., 1998). The flexibility of neural networks allows us to investigate and implement PTFs that use limited or more expanded sets of input variables to predict hydraulic properties.

All PTFs provide estimates of soil hydraulic properties. Considerable scatter exists between measurements and predictions of various PTFs, as shown by Tietje and Tapkenhinrichs (1993); Kern (1995) and Tietje and Hennings (1996). The reliability of a PTF can be judged by how well it describes an independent data set. However, predictions may actually be more reliable for certain subsets of the data and less reliable for others. It would be useful if a PTF was able to provide both a prediction and an associated reliability. In this paper we will show some results of predicting water retention, saturated and unsaturated soil hydraulic conductivity with neural networks using different levels of input data. By combining the neural networks with the bootstrap method (Efron and Tibshirani, 1993) we can provide a probabilistic distribution of the predicted parameters.

## 2. Materials and methods

The data for this study were taken from the UNSODA database (Leij et al., 1996) which consists of 791 entries of field and laboratory measured water retention, saturated and unsaturated hydraulic conductivity as well as particle size distribution data and bulk density of many international sources. Sufficient laboratory water retention data were available for 554 samples, a subset of 315 samples had $K_s$ data while of 245 samples reliable $K(h)$ characteristics were available. The water retention and conductivity functions, Eqs. (1),(3) and (4), were fitted independently to the data with the simplex algorithm (Nelder and Mead, 1965). For Eq. (1) this resulted in $\theta_r$, $\theta_s$, $\alpha$ and $\beta$. We fitted $K_s$ in two versions of Eq. (3) by fixing $\delta$ to 0.5 (Mualem, 1976) or $-1.0$ (Schaap and Leij, 1998) and deriving $\beta$ and $S_e$ from Eq. (1). Fitting Eq. (4) resulted in three parameters: $K_s$, $a$ and $b$. Conductivity data were log-transformed to remove bias towards high conductivities.

Neural network models were calibrated to predict the fitted hydraulic parameters and the measured $K_s$ values from soil texture, bulk density and water retention points. Four levels of input variables were used: (i) sand, silt and clay (SSC); (ii) SSC with the addition of bulk density (SSCBD); (iii) SSCBD with one retention point at 33 kPa (SSCBD$\theta_{33}$) and (iv) SSCBD with retention points at 10 and 33 kPa SSCBD$\theta_{10}\theta_{33}$.

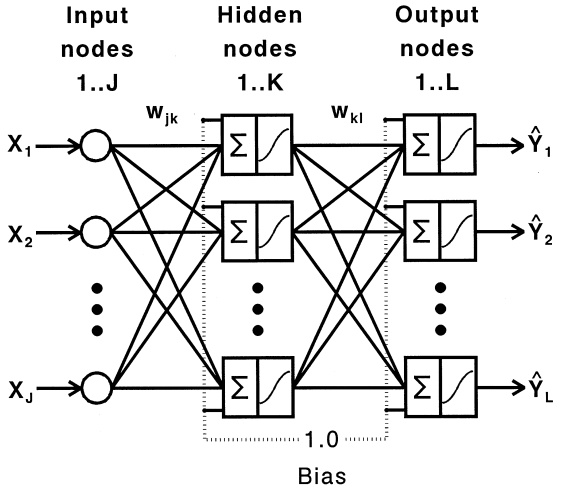


Fig. 1. Schematic overview of a three-layer neural network.

The usage of more input variables is expected to improve the predictions. Still, the simpler models are useful because they can be used when, for example, only the soil texture is known. The hierarchical approach followed here thus adds a degree of flexibility in estimating soil hydraulic properties. Because the particle size information is based on only three classes, the models can predict only mono-modal pore size distributions.

The neural networks that were used in this study consist of an input, a hidden and an output layer all containing 'nodes' (Fig. 1). The numbers of nodes in input and output layers correspond to the number of input and output variables of the model. After Schaap and Bouten (1996), we used six hidden nodes. All input nodes $j$=1...$J$, with the input variables $x_1 \ldots x_J$, are connected to all hidden layer nodes $k$=1...$K$ by means of the adaptable connections, or "weights", $w_{jk}$ which can vary between $-\infty$ and $\infty$. At the hidden nodes, the input values and weights are multiplied and summed Eq. (5) the result, $S_k$, is input into a sigmoid function Eq. (6) yielding the hidden node output $H_k$.

$$S_k = \sum_{j=0}^{J} (w_{jk} \times x_j) \tag{5}$$

$$H_k = \frac{1}{1 + e^{-s_k}} \tag{6}$$

A bias value $x_0$ (equal to 1) and weights $w_{0k}$ are used to offset $S_k$. The output nodes $l$=1...$L$ operate in the same way as the hidden nodes. The hidden node outputs, $H_k$, are multiplied by the weights $w_{kl}$ and the model outputs ($\hat{Y}_l$) are produced in the same way as in $H_k$ in Eq. (6). The values of $w_{jk}$ and $w_{kl}$ are obtained in an iterative calibration procedure.

The neural network calibrations were combined with the bootstrap (Efron and Tibshirani, 1993) to generate uncertainty estimates and to test the neural networks on independent data. Briefly, the bootstrap creates multiple random subsets of the original dataset by sampling with replacement. Each sample thus has a chance of $1 - [(N-1)/N]^N$ to be selected once or multiple times for a particular subset resulting in subsets that contain about 63% of the original data. On each subset a neural network calibration was performed leading to a submodel which was subsequently tested on the 37% of the data that were not present in the subset. Because each subset contains slightly different data, slightly different submodels result. The predictions of the submodels are averaged to yield the model prediction for a hydraulic property. The standard deviation of the submodel predictions provides the uncertainty of a model prediction as a probability density function. The reader is referred to Efron and Tibshirani (1993) and Schaap et al. (1998) for a more thorough description of this method. The combined neural network-bootstrapping analysis was carried out with a slightly adapted TRAINLM routine of the neural network toolbox (version 2.0) of the MATLAB®[1] package (version 4.0, MathWorks, Natick, Massachussets). A maximum of 60 iterations was sufficient for neural network calibration. We used 60 bootstrap subsets to calculate model uncertainty.

Results are presented as root mean square residuals (RMSR) of predicted and measured hydraulic properties of calibration or independent data according to:

$$\mathrm{RMSR} = \sqrt{\frac{1}{N}\sum_{i=1}^{N_t}(Y_i - Y_i')^2} \tag{7}$$

where $N_t$ is the total number of observations for water retention, $K_s$, or unsaturated hydraulic conductivity; $Y_i$ is the measured hydraulic property, $Y_i'$ is the predicted hydraulic property.

[1]Trade names are provided for the benefit of the reader and do not imply endorsement by the USDA.

## 3. Results

Table 1 shows that using more input variables lowers the RMSR values of water retention, saturated and unsaturated conductivity. For water retention, the addition of bulk density and especially one or two water retention points contributed to the predictability. The RMSR for independent data to decreased from 0.107–0.073 $cm^3\ cm^{-3}$. The RMSR of $\log(K_s)$ decreased from 0.840–0.713 $\log(cm\ day^{-1})$. Addition of bulk density or one retention point improved the prediction of $K_s$ whereas using two retention points instead of one decreased the RMSR by only a small margin. RMSR values for all three investigated unsaturated conductivity functions were larger than those for the saturated hydraulic conductivity, reflecting the high error margin with which $K(h)$ measurements are commonly made. The Mualem-van Genuchten model Eq. (3) with $\delta$=0.5 has the highest RMSR for all four input data levels. Using $\delta$=−1.0 instead leads to considerable improvement. The empirical Gardner (1958) model still was somewhat better. All three conductivity models are relatively insensitive to the input data level. Addition of BD and one or two retention points improved the prediction of $K(h)$ only slightly. Inclusion of soil variables other than those discussed here did not improve the prediction of $\theta(h)$, $K_s$ or $K(h)$.

The difference in RMSRs for calibration and independent data was found to be small, thus indicating that the neural network models were rather robust. However, we note that the lowest RMSRs were not nearly as small as the RMSRs of the direct fits of Eqs. (1),(3) and (4) to the data (Table 1). Hence, there must be considerable uncertainty with which the predictions are made. This uncertainty is partly caused by noise in the measurements and partly by the dependence of the models on the calibration data.

The combination of the neural network calibration with the bootstrap method enables us to quantify model uncertainty on a per sample basis. Figs. 2–4 show the uncertainty as predicted by the models that used SSCBD$\theta_{33}$ as input for water retention, $K_s$ and the Gardner function Eq. (4) respectively, for both a loamy sand and a clay sample. For water retention and the Gardner function, 10 and 90% percentiles of the variability among the submodels are shown; for $K_s$ we show the entire probability distribution. Directly apparent from the figures is the larger uncertainty for the clay as compared to the loamy sand. This is caused by the lower number of fine-textured soils in the data set relative to coarse-textured soils. In general, the uncertainty estimates increased when predictions were made for samples that were less common in the calibration data sets.

Table 1
Root mean square residuals (RMSR) for neural network models predicting water retention parameters (VG), saturated hydraulic conductivity $K_s$, and unsaturated conductivity according to van Genuchten (1980) with $\delta$=0.5 and −1.0 (MVG) and Gardner (1958). Also shown are the RMSR values for the direct fits of the functions to the data

| Input | | VG ($cm^3\ cm^{-3}$) | $K_s$ | MVG $\delta$ ($\log(cm\ day^{-1})$)= | | Gardner |
|---|---|---|---|---|---|---|
| | | | | 0.5 | −1.0 | |
| SSC | calibration | 0.109 | 0.831 | 1.76 | 1.36 | 1.23 |
| SSC | independent | 0.107 | 0.840 | 1.77 | 1.37 | 1.25 |
| SSCBD | calibration | 0.096 | 0.761 | 1.70 | 1.29 | 1.15 |
| SSCBD | independent | 0.098 | 0.775 | 1.74 | 1.29 | 1.22 |
| SSCBD$\theta_{33}$ | calibration | 0.077 | 0.680 | 1.65 | 1.25 | 1.13 |
| SSCBD$\theta_{33}$ | independent | 0.080 | 0.720 | 1.69 | 1.29 | 1.20 |
| SSCBD$\theta_{10}\theta_{33}$ | calibration | 0.068 | 0.661 | 1.62 | 1.18 | 1.12 |
| SSCBD$\theta_{10}\theta_{33}$ | independent | 0.073 | 0.713 | 1.65 | 1.24 | 1.18 |
| Direct fit | all data | 0.013 | NA | 1.08 | 0.77 | 0.22 |

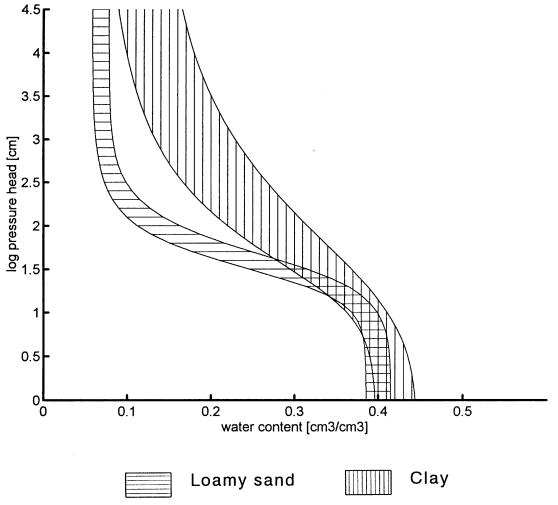


Fig. 2. Ten and 90% uncertainty intervals for water retention as predicted by the SSCBD$\theta_{33}$ model for water retention for a loamy sand.

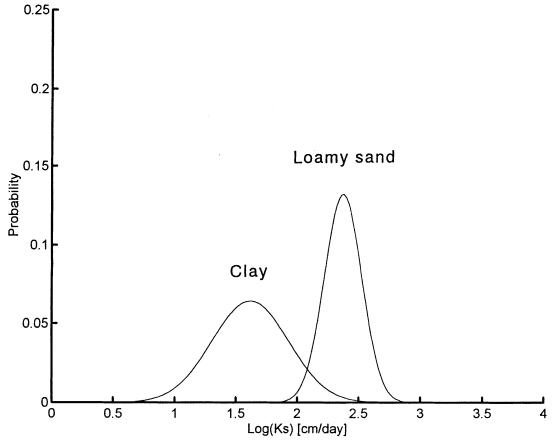


Fig. 3. Uncertainty for $K_s$ as predicted by the SSCBD$\theta_{33}$ model for a loamy sand and a clay.

Note that the saturated hydraulic conductivity in Fig. 3 is higher than the apparent saturated hydraulic conductivity inferred at log($h$)=0 in Fig. 4. This result is consistent with the data in UNSODA. Most $K_s$ measurements include flow through macropores, whereas most $K(h)$ measurements usually exclude macropores by starting at a low suction resulting in empty macropores and a lower 'saturated' conductivity.

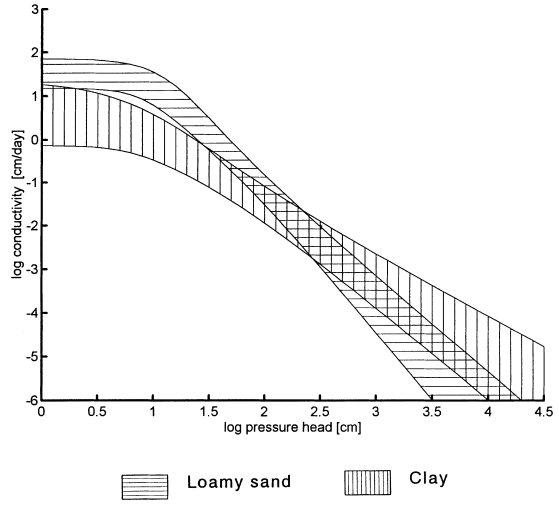


Fig. 4. Ten and 90% uncertainty intervals for unsaturated hydraulic conductivity (Gardner Equation) as predicted by the SSCBD$\theta_{33}$ model for a loamy sand.

## 4. Conclusion

This paper focussed on the prediction of hydraulic properties that are required to solve the Richards equation. We created an hierarchical system of neural network models that predict soil hydraulic properties from different levels of input data. Because all models were calibrated with data from one database the predictions among models and input data levels are consistent. Additionally, the availability of uncertainty estimates provided information about the reliability of the predictions. These characteristics can be very useful to generate uncertainty estimates of water and solute transport processes, even when limited information about the soil is available. Although prediction errors and confidence limits were often large, estimation of soil hydraulic properties with PTFs may be accurate enough for most applications, and hence will fill a need where hydraulic properties are not readily available.

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