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# DIVISION S-1—SOIL PHYSICS

## Neural Network Analysis for Hierarchical Prediction of Soil Hydraulic Properties

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### ABSTRACT

**The solution of many field-scale flow and transport problems requires estimates of unsaturated soil hydraulic properties. The objective of this study was to calibrate neural network models for prediction of water retention parameters and saturated hydraulic conductivity, $K_s$, from basic soil properties. Twelve neural network models were developed to predict water retention parameters using a data set of 1209 samples containing sand, silt, and clay contents, bulk density, porosity, gravel content, and soil horizon as well as water retention data. A subset of 620 samples was used to develop 19 neural network models to predict $K_s$. Prediction of water retention parameters and $K_s$ generally improved if more input data were used. In a more detailed investigation, four models with the following levels of input data were selected: (i) soil textural class, (ii) sand, silt, and clay contents, (iii) sand, silt, and clay contents and bulk density, and (iv) the previous variables and water content at a pressure head of 33 kPa. For water retention, the root mean square residuals decreased from 0.107 for the first to 0.060 $m^3\ m^{-3}$ for the fourth model while the root mean square residual $K_s$ decreased from 0.627 to 0.451 log(cm $d^{-1}$). The neural network models performed better on our data set than four published pedotransfer functions for water retention (by $\approx$0.01–0.05 $m^3\ m^{-3}$) and better than six published functions for $K_s$ (by $\approx$0.1–0.9 order of magnitude). Use of the developed hierarchical neural network models is attractive because of improved accuracy and because it permits a considerable degree of flexibility toward available input data.**

CONCERN ABOUT THE QUALITY of soil and water resources has motivated the development of increasingly sophisticated models for predicting water flow and solute transport in unsaturated soils. These models generally require knowledge of the soil water retention, $\theta(h)$, and unsaturated hydraulic conductivity, $K(h)$, where $\theta$ is the volumetric water content and $h$ is the pressure head. Direct measurement of these properties is often time consuming and expensive, while the results may not be accurate. An alternative is the use of pedotransfer functions (PTFs), which estimate the hydraulic properties through correlation with more easily measured or widely available soil parameters (Bouma and van Lanen, 1987; van Genuchten and Leij, 1992).

A variety of PTFs with different mathematical concepts, predicted properties, and input data requirements have been developed. Quasi-physical methods by Arya and Paris (1981), Haverkamp and Parlange (1986), and Tyler and Wheatcraft (1989) use the concept of shape similarity between pore- and particle-size distributions. The vast majority of PTFs, however, are empirically based on relatively simple linear regression equations. Although considerable differences exist among PTFs in terms of the required input data, all of them use at least some information about the particle-size distribution. When only the textural classification is known, simple "class" PTFs can be used to provide average hydraulic properties for each soil textural class (Carsel and Parrish, 1988; Wösten et al., 1995). When the actual particle-size distribution is known, PTFs that predict continuously changing hydraulic properties across the textural triangle can be used.

Pedotransfer function predictions may be improved by extending the input data through addition of basic soil properties like bulk density, porosity, or organic matter content (Rawls and Brakensiek, 1985; Vereecken et al., 1989). Additional improvements may be achieved by including one or more water retention data points (Rawls et al., 1992; Williams et al., 1992). Ahuja et al. (1989) and Messing (1989) similarly improved predictions of saturated hydraulic conductivity, $K_s$, by using effective porosity data, which they defined as the total porosity minus the water content at 10 or 33 kPa pres-

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**Abbreviations:** PTF, pedotransfer function; $\rho_b$, bulk density; $EP_{10}$, effective porosity at 10 kPa; $EP_{33}$, effective porosity at 33 kPa; $EP_{1500}$, effective porosity at 1500 kPa; HOR, horizon; POR, porosity; PTF, pedotransfer function; RMSR, root mean square residual, Eq. [4] and [5]; SSC, sand, silt, clay content; TXT, textural class.

sure head. Other researchers have predicted soil hydraulic properties using more limited or extended sets of input variables (Rawls et al., 1992; Schaap and Bouten, 1996; Vereecken et al., 1989, 1990). Such hierarchical approaches are of great practical use since they permit more flexibility toward the required input data when predicting the hydraulic properties.

Neural-network-based PTFs were recently used by Pachepsky et al. (1996), Schaap and Bouten (1996), and Tamari et al. (1996). The feed-forward backpropagation or radial basis functions used by these researchers are able to approximate any continuous (nonlinear) function to any desired degree of accuracy (Hecht-Nielsen, 1990; Haykin, 1994). An advantage of neural networks, compared with traditional PTFs, is that neural networks require no a priori model concept. The optimal relations that link input data (basic soil properties) to output data (hydraulic parameters) are obtained and implemented in an iterative calibration procedure. For a data set of 204 sandy soil samples, Schaap and Bouten (1996) showed that neural networks made predictions with significantly smaller errors than more traditional linear regression approaches. Pachepsky et al. (1996) used a data set of 230 soil samples. They found that neural networks predicted water retention points better than multilinear regression, but that the two methods produced comparable results when water retention parameters were predicted. Tamari et al. (1996) used synthetic $K(h)$ data sets and found that neural networks were not better than multilinear regression models if the uncertainty in the data was large. The neural networks performed better than regression when real soil data were used.

It was the objective of this study to predict van Genuchten (1980) water retention parameters and saturated hydraulic conductivity for a hierarchical input structure. The corresponding sequence of neural network PTFs yields a collection of models of which the most suitable one can be selected depending on the available basic soil properties. We also used neural networks to establish which basic soil properties are the most relevant for predicting the hydraulic properties. Contrary to previous work on neural network PTFs, a data set was employed that covers most of the textural triangle, thus ensuring broad applicability of the hierarchical approach. Conventional error criteria and independent data were used to evaluate the performance of the hierarchical neural network models, and to test performance of previously published PTFs. The uncertainty in the predicted soil hydraulic properties was evaluated by combining the neural network approach with the bootstrap method (Efron and Tibshirani, 1993).

## MATERIALS AND METHODS

### Data Set

The data set for calibration and testing was extracted from a database consisting of 4515 laboratory samples taken from about 30 sources in the USA (W.J. Rawls, USDA-ARS Hydrology Lab., Beltsville, MD, 1996, personal communication). We selected 1209 samples for water retention (containing six to 13 points with different pressure head ranges), soil texture, and bulk density; a subset of 620 samples had $K_s$ measurements. Figures 1a and 1b show the distributions of the samples in the USDA textural triangle for the entire 1209-sample data set and the $K_s$ subset. For subsequent analysis, the samples in the sandy clay, clay, and silty clay classes were grouped into one class ("clays"); silt and silt loam classes were grouped into "silts"; 405 samples were from A horizons, 588 from B horizons, and 216 from C horizons.

Water retention data for each of the 1209 samples were fitted to the van Genuchten (1980) equation:

$$\theta(h) = \theta_r + \frac{\theta_s - \theta_r}{[1 + (\alpha h)^n]^m} \quad [1]$$

where $\theta_s$ and $\theta_r$ are saturated and residual water contents respectively; $\alpha$ ($cm^{-1}$) and $n$ are curve shape parameters, and following van Genuchten (1980), $m = 1 - 1/n$. Fitting was carried out with the simplex or amoeba algorithm (Nelder

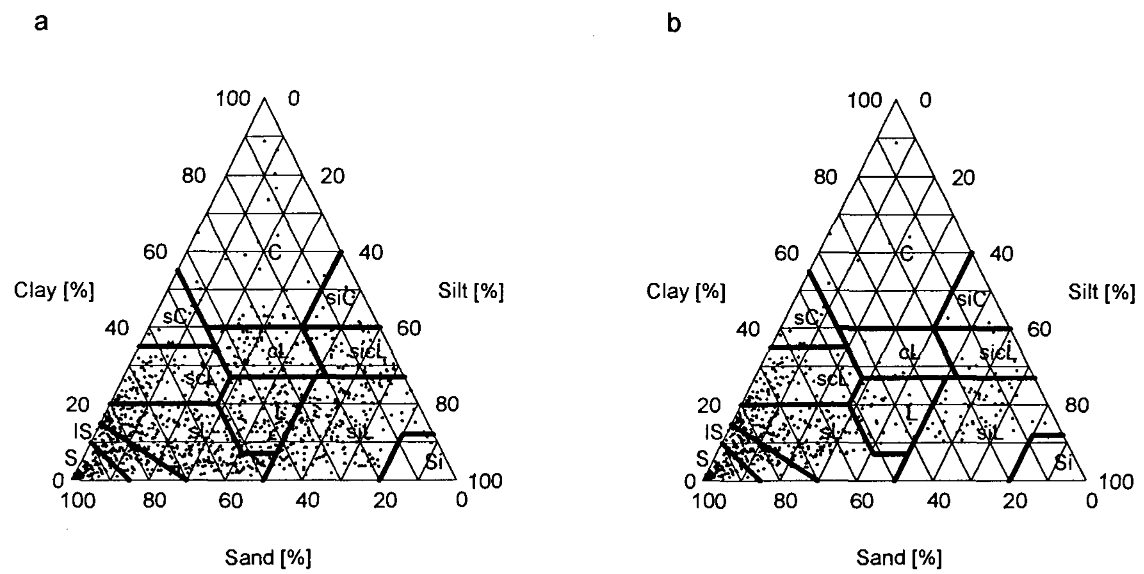


**Fig. 1. Textural distribution of the (a) water retention data set and the (b) saturated hydraulic conductivity ($K_s$) subset. S: sand, C: clay, Si: silt, L: loam, s: sandy, c: clayey, si: silty, l: loamy.**

and Mead, 1965; Press et al., 1988) with the following constraints: $0.0 \leq \theta_r \leq 0.3$ m$^3$ m$^{-3}$, $0.6\phi \leq \theta_s \leq \phi$ m$^3$ m$^{-3}$ (where $\phi$ is the total porosity), $0.0001 \leq \alpha \leq 1.000$ cm$^{-1}$, and $1.001 \leq n \leq 10$. The parameters $\alpha$ and $n$ were then log-transformed to obtain approximately normal distributions. The same transformation was also carried out for $K_s$ measurements.

## Published Pedotransfer Functions

In this study we used four previously published PTFs to predict water retention parameters (R1 through R4 in Table 1) and six published PTFs to predict saturated hydraulic conductivity (K1 through K6 in Table 2). Tables 1 and 2 also show the required input data for each PTF. All PTFs consist of the same coefficients and variables as in the original publications. We did not recalibrate the PTFs for our data set because of their empirical nature. Recalibration would not only require adaption of the coefficients but also an evaluation of whether the input variables or expressions used are actually appropriate for the current data set. Recalibration might have resulted in completely different PTFs than were published.

The R1 and R3 functions predicted parameters of the Brooks and Corey (1964) water retention function, given by:

$$\theta(h) = \theta_{r,BC} + (\theta_{s,BC} - \theta_{r,BC})\left(\frac{h_b}{h}\right)^{\lambda} \quad [2]$$

where $h_b$ is the air-entry pressure and $\lambda$ is an empirical parameter. The function R1 (Rawls and Brakensiek, 1985) assumed that the saturated water content, $\theta_{s,BC}$, is equal to the porosity. The function R3 (Cosby et al., 1984) predicted Brooks–Corey parameters according to Campbell (1974), i.e., with $\theta$ as the independent variable and $\theta_{r,BC} = 0$.

The R2 and R4 functions predicted parameters of Eq. [1]. In R2, Rawls and Brakensiek (1985) transformed the Brooks–Corey parameters as predicted by R1 into the van Genuchten (1980) parameters using the expressions in Table 1. For R4, $m$ in Eq. [1] is set to 1 (Vereecken et al., 1989).

Functions K1, K2, and K4 (Table 2) provide relatively straightforward expressions between $K_s$ and the listed soil properties. Function K3 of Saxton et al. (1986) predicts a $K(\theta)$ relationship using sand and clay contents. Substitution of the total porosity, $\phi$, for $\theta$ yields an estimate for $K_s$. The coefficient of determination of this PTF is very high ($R^2 = 0.95$, Saxton et al., 1986) since it was fitted to predictions of a PTF reported earlier by Rawls et al. (1982). Function K5 by Ahuja et al. (1989) expresses $K_s$ as a power function of effective porosity parameter ($EP_{33}$, calculated from the total porosity minus the water content, $\theta_{33}$, at 33 kPa). As parameter values in this power function we used 1015 for the multiplication factor and 4.0 for the exponent as suggested by Rawls et al. (1992). Finally, K6 is a quasi-physical PTF by Mishra and Parker (1989, 1992) that calculates $K_s$ based on closed-form expressions by Mualem (1976), Brutsaert (1968), and van Genuchten (1980).

**Table 1. Input and output data of four pedotransfer functions (PTF) that predict selected soil water retention parameters.**

| PTF | Input | Output | $R^2_{calib}$† |
|---|---|---|---|
| R1 Rawls and Brakensiek (1985) | | Eq. [2] | |
| | Sand, clay, $\phi$ | $\theta_{r,BC}$ | NA |
| | $\phi$ | $\theta_{s,BC}$ | NA |
| | Sand, clay, $\phi$ | $h_b$ | NA |
| | Sand, clay, $\phi$ | $\lambda$ | NA |
| R2 Rawls and Brakensiek (1985) | | Eq. [1], $m = 1 - 1/n$ | |
| | $\theta_r = \theta_{r,BC}$ | $\theta_r$ | NA |
| | $\theta_s = \theta_{s,BC}$ | $\theta_s$ | NA |
| | $\alpha = 1/h_b$ | $\alpha$ | NA |
| | $n = \lambda + 1$ | $n$ | NA |
| R3 Cosby et al. (1984) | | Eq. [2], $\theta_{r,BC} = 0$ | |
| | Sand | $\theta_{s,BC}$ | 0.771 |
| | Sand | $h_b$ | 0.809 |
| | Clay | $\lambda$ | 0.966 |
| R4 Vereecken et al. (1989) | | Eq. [1], $m = 1$ | |
| | Clay, $\rho_b$ | $\theta_r$ | 0.703 |
| | Clay, Organic C | $\theta_s$ | 0.848 |
| | Sand, clay, $\rho_b$, Organic C | $\alpha$ | 0.680 |
| | Sand, clay | $n$ | 0.560 |

† Published coefficient of determination for calibration; NA = not available.

## Neural Network Models

Since several textbooks on neural networks are available (e.g., Hecht-Nielsen, 1990; Haykin, 1994), we provide only a brief summary of the neural network approach. In this study we used a back-propagation neural network with one hidden layer. This type of neural network is a nonlinear data transformation structure consisting of input and output nodes connected to a number of hidden nodes by adaptable coefficients. The number of input and output nodes corresponds to the number of input and output variables. The number of hidden nodes depends on the complexity of the underlying problem and is determined empirically by calibrating neural networks with different numbers of hidden nodes. After Schaap and Bouten (1996), we used six hidden nodes. Both the hidden and output nodes contain sigmoidal transfer functions that provide the neural network with nonlinear capabilities. The coefficients were obtained in an iterative calibration procedure based on, in our case, the Levenberg–Marquardt algorithm (Marquardt, 1963). This algorithm minimizes the objective function:

$$O(t,t') = \sum_{i=1}^{N_t} \sum_{j=1}^{N_c} (t_{i,j} - t'_{i,j})^2 \quad [3]$$

where $t$ and $t'$ are the measured and predicted output variables, $N_c$ is the total number of calibration samples, $N_t$ is the total number of hydraulic parameters (one for $K_s$ and four for the retention parameters in Eq. [1]).

A neural network model obtained in the calibration procedure should always be tested on independent data. Usually this is done by calibrating the neural network on one part of a data set and subsequently testing the network on the other part. We followed this approach, and also estimated uncertainty in neural network predictions by combining multiple

**Table 2. Input and output data of six pedotransfer functions (PTFs) that predict the saturated hydraulic conductivity, $K_s$.**

| PTF | Input data | Output | $R^2_{calib}$† |
|---|---|---|---|
| K1 Cosby et al. (1984) | Sand | $K_s$ | 0.839 |
| K2 Brakensiek et al. (1984) | Sand, clay, $\phi$ | $K_s$ | NA |
| K3 Saxton et al. (1986) | Sand, clay, $\theta$ | $K(\theta)$‡ | 0.95 |
| K4 Vereecken et al. (1990) | Sand, clay, $\rho_b$, Organic C | $K_s$ | 0.20 |
| K5 Ahuja et al. (1989) | Effective porosity at 33 kPa | $K_s$ | 0.33–0.71§ |
| K6 Mishra and Parker (1991) | $\theta_r$, $\theta_s$, $\alpha$ | $K_s$ | NA |

† Published coefficient of determination for calibration; NA = not available.
‡ See text for explanation.
§ Ahuja et al., 1989.

calibration and testing runs with the bootstrap method (Efron and Tibshirani, 1993).

The bootstrap method is a nonparametric technique for calculating the probability distribution of any statistic, in our case hydraulic parameters as predicted by neural networks. The bootstrap does not make assumptions about the shape of the distribution of the underlying population, nor does it matter how complex is the calculation of the statistic (Efron and Tibshirani, 1993). It is assumed that the data set involved is a good representation of the original population with the understanding that this data set is only one particular realization of that population. Calibration of a model on another realization would therefore always lead to slightly different predictions of $\theta_r$, $\theta_s$, $\alpha$, $n$, and $K_s$ and thus cause uncertainty about the true value of these parameters. Unfortunately, we often have only one realization of the population. Bootstrapping simulates different realizations by repeated random resampling with replacement of the original data set of size $N$ to yield $B$ bootstrap data sets of size $N$. Each bootstrap data set contains somewhat different data, which results in $B$ neural network models, all of which may differ slightly. Efron and Tibshirani (1993) suggested $B$ to be between 50 and 200; we used $B = 60$.

Because resampling is done with replacement, each sample has a chance of $1 - [(N - 1)/N]^N$ (approximately 63%) to be selected once or multiple times for a bootstrap data set. Each bootstrap data set thus contains one or more copies of 63% of the samples. Although formally not part of the bootstrap method, the remaining 37% of the samples can be used to carry out an independent test (cf. Efron and Tibshirani, 1993, p. 252–254). By calculating averages and standard deviations of $B$ testing results, one obtains robust values of the predicted hydraulic parameters and associated uncertainty estimates for independent data.

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 Inc., Natick, MA) and default optimization parameters. By plotting the error evolution vs. the number of iterations, we found that 50 iterations were generally enough to find the minimum in $O(t,t')$. In a limited number of calibrations, a local minimum was found [$O(t,t')$ was larger than twice the average minimum value]. In those cases the neural network calibration procedure was restarted with a different set of random initial weights. Depending on the neural network model, about six to 24 h on a P5-166 MHz PC were required for calibration. Testing the calibrated neural network models with independent data needed only a few seconds.

## Hierarchical Approach

Two series of 12 water retention and 19 $K_s$ neural network models were developed in a hierarchical approach using input data listed in the first column of Table 4. The first 12 $K_s$ models use exactly the same input data as the retention models; the last seven $K_s$ models use input data that are not considered for the retention models.

First, we carried out analyses using minimal input data, i.e., only textural class information (TXT in Table 4) similar to the class PTFs of Carsel and Parrish (1988) and Wösten et al. (1995). Next, neural networks were developed that used sand, silt, and clay fractions as input (SSC). Although one of these fractions always contains redundant information, we used all three as input to allow the neural network to select the most relevant variable. In a subsequent model, bulk density ($\rho_b$) was added to the input variables (SSC$\rho_b$). Next, we substituted porosity (POR) for $\rho_b$ (SSCPOR). Since bulk density and porosity are closely related, the change in input variable was not expected to greatly affect the results. Information was added about the gravel content (particle size >2 mm) to yield the SSC$\rho_b$+Gravel model or the horizon information to give SSC$\rho_b$ + HOR model. Horizon information was encoded as one variable (HOR) with A horizons as 0, B horizons as 0.5, and C horizons as 1.

Subsequent neural network models also considered one or several input variables derived from retention data. Although it was the purpose of this study to predict retention parameters and $K_s$, limited retention measurements are sometimes available (cf. Soil Survey Staff, 1995). Assimilation of available retention data in PTFs may improve the prediction of hydraulic properties (e.g., Rawls et al., 1992). Seven models used the same input variables as the SSC$\rho_b$ model, but with addition of one or two retention points ($\theta_{10}$, $\theta_{33}$, and $\theta_{1500}$ at $h$ = 10, 33, and 1500 kPa, respectively; see Table 4). The water contents were obtained by evaluating the fitted retention parameters of Eq. [1] at the appropriate pressure heads.

Four additional neural network models were developed for $K_s$ using the same input as the SSC$\rho_b$ model and effective porosity (i.e., SSC$\rho_b$ + EP$_{10}$, SSC$\rho_b$ + EP$_{33}$, and SSC$\rho_b$ + EP$_{1500}$ models) or estimated retention parameters (SSC$\rho_b$ + $\theta_r\theta_s\alpha n$). Effective porosity was calculated by subtracting the water content at the appropriate pressure head (10, 33, or 1500 kPa) from the total porosity. Following Ahuja et al. (1989) and Messing (1989), we also tried to predict $K_s$ from EP$_{10}$ or EP$_{33}$, exclusively. Finally, we attempted to predict $K_s$ using only retention parameters ($\theta_r$, $\theta_s$, $\alpha$, $n$) so as to allow a comparison with the PTF of Mishra and Parker (1989, 1992).

We evaluated TXT, SSC, SSC$\rho_b$, and the SSC$\rho_b$+$\theta_{33}$ models by textural class because they appeared to be the most useful models for practical applications.

## Evaluation Criteria

The neural network predictions were evaluated in terms of the coefficient of determination ($R^2$) between predicted and fitted or measured hydraulic parameters ($\theta_r$, $\theta_s$, $\alpha$, $n$, and $K_s$). We did not evaluate the published water retention PTFs in this way since most predict parameters for functions other than Eq. [1]. Additionally, we compared the predictions of the neural networks and the published PTFs with measured data as root mean square residuals (RMSR$_{wrc}$ and RMSR$_{K_s}$). The RMSR$_{wrc}$ was obtained by converting the predicted parameters to water contents at the appropriate pressure heads and calculating:

$$\mathrm{RMSR}_{wrc} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\frac{\sum_{j=1}^{L}(\theta_{i,j} - \theta'_{i,j})^2}{L - n_{par}}} \qquad [4]$$

where $N$ is the number of samples (1209), $L$ the number of measured retention points for each sample, $\theta_{i,j}$ and $\theta'_{i,j}$ are measured and predicted water retention points, and $n_{par}$ is the number of parameters (four). The root mean square residual for log($K_s$) was similarly calculated as:

$$\mathrm{RMSR}_{K_s} = \sqrt{\frac{1}{M}\sum_{j=1}^{M}[\log(K_s) - \log(K'_s)]^2} \qquad [5]$$

where $M$ is the number of samples (620), while log($K_s$) and log($K'_s$) denote measured and predicted values, respectively.

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

For all models in the hierarchical approach listed in Table 4, we present average $R^2$ and RMSR values of the 60 bootstrap models. The variability of the bootstrap predictions will be quantified by standard deviations (the predicted parameters had approximately normal distributions). The RMSR results of published PTFs were calculated for the entire data set of 1209 water retention samples or the 620-sample $K_s$ subset without bootstrapping. Applying the bootstrap to evaluate the published PTFs is not useful because, contrary to the neural networks, these models stay the same for all bootstrap data sets.

## RESULTS AND DISCUSSION

The results of the direct fit of Eq. [1] to retention data for each textural class (Table 3) are generally similar to those reported by Carsel and Parrish (1988) with the following exceptions. The average $\theta_s$ values were lower for loam (0.356 m$^3$ m$^{-3}$ for our data vs. 0.43 m$^3$ m$^{-3}$ for Carsel and Parrish [1988]) and higher for clays (0.441 vs. 0.38 m$^3$ m$^{-3}$). Further, the values for log($\alpha$) were generally lower because we calculated the average of log($\alpha$), but Carsel and Parrish (1988) computed the average of $\alpha$. For example, for the loam class we found log($\alpha$) to be $-2.11$ log(cm$^{-1}$) while Carsel and Parrish (1988) found $-1.29$ log(cm$^{-1}$). We also found higher values for $K_s$ for the silty clay loam class [0.87 vs. 0.22 log(cm d$^{-1}$)] and the clays [1.10 vs. 0.68 log(cm day$^{-1}$)]. The average RMSR$_{wrc}$ of the direct fit varies from 0.010 to 0.025 m$^3$ m$^{-3}$ for sandy clay loam and silts, respectively; for the entire data set it was 0.020 m$^3$ m$^{-3}$.

The results of the hierarchical approach (Table 4) show an increase in the $R^2$ and a decrease in RMSR$_{wrc}$ and RMSR$_{Ks}$ if more input variables are used. There is a substantial variation among the different output variables. The behavior of $R^2$ is discussed first.

All neural network models show a low $R^2$ for $\theta_r$; this indicates that $\theta_r$ could not be predicted well from the available input data. A reason for this poor performance is probably the asymptotic nature of $\theta_r$, which is an extrapolated water content at infinite suction while the highest suction available in most cases was not more than 1500 kPa. The mean and standard deviation of the fitted $\theta_r$ in Table 3 suggest a large coefficient of variation in each soil textural class. Table 4 shows that when $\theta_{1500}$ was included in the input, the correlation remained poor: the maximum $R^2$ was 0.41 (SSC$\rho_b$+$\theta_{33}\theta_{1500}$). Schaap and Bouten (1996) also found poor correlations between predicted and fitted $\theta_r$ values. Vereecken et al. (1989) found much higher $R^2$ values (0.70) for $\theta_r$ for a range of Belgian soils while the predicted $\theta_r$ values tended to be higher than our class averages because of a somewhat different retention function by setting $m = 1$ in Eq. [1].

A comparison of $R^2$ for $\theta_s$ of the TXT and SSC models with those of the SSC$\rho_b$ and SSCPOR models shows that information about the soil bulk density is important for accurately predicting $\theta_s$. If only basic soil properties were used to predict $\theta_s$, the maximum $R^2$ was 0.63 (SSC$\rho_b$ + Gravel). If water contents were used as additional input, $R^2$ increased to 0.68 for the SSC$\rho_b$ + $\theta_{10}$ neural network model, and to 0.77 for the SSC$\rho_b$ + $\theta_{10}\theta_{33}$ model.

The results for log($\alpha$) and log($n$) were rather similar. A slight increase in $R^2$ is noticeable for the SSC model, compared with the TXT model. Correlations were between 0.35 and 0.40 if only basic soil properties were used. The addition of horizon information or gravel to the input did not improve the prediction, nor did the replacement of $\rho_b$ with porosity (POR). Addition of $\theta_{10}$ or $\theta_{33}$ to the input improved the correlations to 0.58 for both log($\alpha$) and log($n$) (SSC$\rho_b$ + $\theta_{33}$ model) and to 0.65 for log($\alpha$) and 0.70 for log($n$) if both $\theta_{10}$ and $\theta_{33}$ were used (SSC$\rho_b$ + $\theta_{10}\theta_{33}$ model). The $\theta_{1500}$ variable did not provide useful information for predicting log($\alpha$) or log($n$).

The correlation for log($K_s$) improved if the SSC model was used instead of TXT; further improvement was achieved with the SSC$\rho_b$ model (Table 4). Addition of gravel or horizon information or replacing $\rho_b$ with POR did not significantly improve the correlation. The maximum correlation that could be obtained with basic soil properties alone was 0.58. Including information derived from the water retention data improved the correlation to as much as 0.72 (SSC$\rho_b$ + EP$_{10}$). Information contained in $\theta_{1500}$ was apparently not as useful as adding $\theta_{10}$ and $\theta_{33}$ or EP$_{10}$ and EP$_{33}$. Notice that the results for the SSC$\rho_b$ + $\theta_{10}$ and SSC$\rho_b$ + $\theta_{33}$ models were very similar to those for the SSC$\rho_b$ + EP$_{10}$ and SSC$\rho_b$ + EP$_{33}$ models. This finding is not surprising since the input data were essentially the same (porosity can be derived from bulk density while effective porosity can be calculated from porosity and water content). Using only EP$_{10}$ or EP$_{33}$ as input, as was done by Ahuja et al. (1989)

**Table 3. Average values and standard deviations ($\sigma$, in parentheses) of fitted hydraulic parameters, root mean square residuals (RMSR), and the number of samples for nine textural classes.**

| Class | $N_{wrc}$† | $\theta_r$ | $\theta_s$ | log($\alpha$) | log($n$) | RMSR$_{wrc}$ | $N_{Ks}$† | $K_s$ |
|---|---|---|---|---|---|---|---|---|
| | | m$^3$ m$^{-3}$ | m$^3$ m$^{-3}$ | log(cm$^{-1}$) | | m$^3$ m$^{-3}$ | | log (cm d$^{-1}$) |
| Sand | 97 | 0.044 (0.019) | 0.413 (0.057) | −1.57 (0.21) | 0.462 (0.200) | 0.019 | 97 | 2.71 (0.51) |
| Loamy sand | 135 | 0.039 (0.037) | 0.395 (0.072) | −1.49 (0.53) | 0.194 (0.108) | 0.018 | 117 | 1.92 (0.61) |
| Sandy loam | 337 | 0.031 (0.049) | 0.389 (0.094) | −1.57 (0.58) | 0.150 (0.094) | 0.021 | 199 | 1.53 (0.65) |
| Loam | 137 | 0.054 (0.067) | 0.356 (0.082) | −2.11 (0.82) | 0.195 (0.140) | 0.017 | 32 | 0.99 (0.63) |
| Silts‡ | 220 | 0.065 (0.062) | 0.441 (0.103) | −2.51 (0.49) | 0.260 (0.131) | 0.025 | 62 | 1.04 (0.54) |
| Sandy clay loam | 104 | 0.076 (0.074) | 0.379 (0.066) | −1.80 (0.66) | 0.132 (0.100) | 0.010 | 80 | 1.29 (0.70) |
| Clay loam | 77 | 0.091 (0.067) | 0.439 (0.077) | −1.95 (0.60) | 0.188 (0.128) | 0.016 | 6 | 0.67 (0.58) |
| Silty clay loam | 47 | 0.111 (0.062) | 0.460 (0.056) | −2.36 (0.38) | 0.240 (0.110) | 0.015 | 10 | 0.87 (0.55) |
| Clays§ | 55 | 0.081 (0.088) | 0.441 (0.068) | −1.89 (0.55) | 0.107 (0.059) | 0.014 | 17 | 1.10 (0.43) |

† Total 1209 samples for water retention and 620 for $K_s$.
‡ Silt and silty loam.
§ Clay, silty clay, and sandy clay.

**Table 4. Average values and standard deviations ($\sigma$, in parentheses) of coefficients of determination ($R^2$) and root mean square residuals ($RMSR_{wrc}$ for water retention and $RMSR_{Ks}$ for $K_s$) for 12 models that predict retention parameters and 19 models that predict $K_s$. These results are evaluations of the models on independent data.**

| Model input† | $R^2$ | | | | | $RMSR_{wrc}$ | $RMSR_{Ks}$ |
|---|---|---|---|---|---|---|---|
| | $\theta_r$ | $\theta_s$ | log($\alpha$) | log($n$) | log($K_s$) | $m^3$ $m^{-3}$ | log(cm $d^{-1}$) |
| TXT | 0.12 (0.03) | 0.11 (0.02) | 0.29 (0.03) | 0.32 (0.05) | 0.42 (0.04) | 0.107 (0.004) | 0.627 (0.025) |
| SSC | 0.16 (0.05) | 0.10 (0.02) | 0.35 (0.04) | 0.37 (0.05) | 0.47 (0.04) | 0.104 (0.006) | 0.602 (0.026) |
| SSC$\rho_b$ | 0.18 (0.04) | 0.54 (0.04) | 0.38 (0.04) | 0.38 (0.05) | 0.57 (0.04) | 0.087 (0.005) | 0.533 (0.024) |
| SSCPOR | 0.19 (0.04) | 0.53 (0.04) | 0.37 (0.04) | 0.39 (0.04) | 0.57 (0.04) | 0.087 (0.004) | 0.536 (0.025) |
| SSC$\rho_b$ + Gravel | 0.21 (0.05) | 0.63 (0.03) | 0.39 (0.04) | 0.40 (0.04) | 0.58 (0.04) | 0.087 (0.006) | 0.539 (0.024) |
| SSC$\rho_b$ + HOR | 0.17 (0.06) | 0.53 (0.04) | 0.36 (0.03) | 0.38 (0.04) | 0.57 (0.04) | 0.087 (0.004) | 0.537 (0.028) |
| SSC$\rho_b$ + $\theta_{10}$ | 0.23 (0.05) | 0.68 (0.03) | 0.55 (0.03) | 0.55 (0.04) | 0.70 (0.03) | 0.065 (0.003) | 0.448 (0.023) |
| SSC$\rho_b$ + $\theta_{33}$ | 0.26 (0.06) | 0.56 (0.03) | 0.58 (0.03) | 0.58 (0.04) | 0.70 (0.03) | 0.060 (0.005) | 0.451 (0.019) |
| SSC$\rho_b$ + $\theta_{1500}$ | 0.35 (0.07) | 0.52 (0.04) | 0.37 (0.04) | 0.39 (0.05) | 0.59 (0.04) | 0.081 (0.004) | 0.529 (0.024) |
| SSC$\rho_b$ + $\theta_{10}\theta_{33}$ | 0.27 (0.05) | 0.77 (0.02) | 0.65 (0.03) | 0.70 (0.04) | 0.70 (0.03) | 0.058 (0.006) | 0.448 (0.019) |
| SSC$\rho_b$ + $\theta_{10}\theta_{1500}$ | 0.38 (0.06) | 0.68 (0.03) | 0.57 (0.04) | 0.57 (0.04) | 0.70 (0.03) | 0.064 (0.005) | 0.447 (0.022) |
| SSC$\rho_b$ + $\theta_{33}\theta_{1500}$ | 0.41 (0.07) | 0.55 (0.03) | 0.63 (0.03) | 0.64 (0.03) | 0.68 (0.04) | 0.061 (0.004) | 0.463 (0.027) |
| SSC$\rho_b$ + $EP_{10}$ | – | – | – | – | 0.72 (0.03) | – | 0.435 (0.019) |
| SSC$\rho_b$ + $EP_{33}$ | – | – | – | – | 0.70 (0.03) | – | 0.452 (0.019) |
| SSC$\rho_b$ + $EP_{1500}$ | – | – | – | – | 0.60 (0.03) | – | 0.523 (0.024) |
| SSC$\rho_b$ + $\theta_r\theta_s\alpha n$ | – | – | – | – | 0.68 (0.03) | – | 0.467 (0.024) |
| $EP_{10}$ | – | – | – | – | 0.67 (0.03) | – | 0.479 (0.021) |
| $EP_{33}$ | – | – | – | – | 0.65 (0.04) | – | 0.494 (0.025) |
| $\theta_r\theta_s\alpha n$ | – | – | – | – | 0.62 (0.03) | – | 0.504 (0.022) |

† TXT = textural class; SSC = sand, silt, clay contents; $\rho_b$ = bulk density; HOR = horizon; $\theta_{10}$, $\theta_{33}$, $\theta_{1500}$ = water content at 10 kPa, 33 kPa, and 1500 kPa; $EP_{10}$, $EP_{33}$, $EP_{1500}$ = effective porosity at 10 kPa, 33 kPa, and 1500 kPa; $\theta_r$, $\theta_s$, $\alpha$, $n$ = retention parameters in Eq. [2].

and Messing (1989), reduced the effectiveness of the predictions somewhat compared with the SSC$\rho_b$ + $EP_{10}$ or SSC$\rho_b$ + $EP_{33}$ $K_s$ models. The same was true if only van Genuchten (1980) parameters were used (cf. $\theta_r\theta_s\alpha n$ and SSC$\rho_b$ + $\theta_r\theta_s\alpha n$ models), similar to the work of Mishra and Parker (1989, 1992). These results show that SSC$\rho_b$ and effective porosity data or fitted van Genuchten (1980) parameters do not convey exactly the same information. Combining basic soil properties with retention data will lead to more accurate predictions.

The RMSR results for the retention models and log($K_s$) models show similar but decreasing trends to the correlations for the individual parameters. The $RMSR_{wrc}$ values were relatively high for the TXT input data; individual water retention data points were predicted with a standard deviation of 0.107 $m^3$ $m^{-3}$ while log($K_s$) was predicted with a $RMSR_{Ks}$ of 0.627 log(cm $d^{-1}$). As observed by Williams et al. (1992) and Rawls et al. (1992), inclusion of a retention point improved the prediction. The use of two retention points did not improve the prediction much ($RMSR_{wrc}$ was 0.060 $m^3$ $m^{-3}$ for SSC$\rho_b$+$\theta_{33}$ compared with 0.058 $m^3$ $m^{-3}$ for SSC$\rho_b$ + $\theta_{10}\theta_{33}$). Although the $RMSR_{wrc}$ values decreased when more input data were used, they remained high at 0.058 $m^3$ $m^{-3}$ (SSC$\rho_b$ + $\theta_{10}\theta_{33}$), which is well above the $RMSR_{wrc}$ of the direct fit of Eq. [1] to the retention data (0.020 $m^3$ $m^{-3}$). The $RMSR_{Ks}$ values decreased to 0.447 log(cm $d^{-1}$) for the SSC$\rho_b$ + $\theta_{10}\theta_{1500}$ model. Notice that $R^2$ and RMSR values do not necessarily provide similar information: a comparison of the SSC$\rho_b$ + $\theta_{33}$ and SSC$\rho_b$ + $\theta_{10}\theta_{33}$ models shows that the $R^2$ values of most retention parameters increased substantially while the $RMSR_{wrc}$ decreased only modestly. The latter error measure is probably of most direct interest.

The standard deviations in Table 4 provide information about the variability of the $R^2$ and RMSR among the predictions of the 60 bootstrap models. The standard deviations were in most cases about 5 to 10% of the average $R^2$ and RMSR values. This implies that models with different performances are obtained when slightly different calibration data sets are used. A *single* calibration, typical for most or all previously published PTFs, would have had a chance of about 95% to be within two standard deviations of the reported average $R^2$ and RMSR values. This result indicates that there is apparently a substantial uncertainty in the predicted hydraulic properties.

## Evaluation of Selected Models by Textural Class

The $RMSR_{wrc}$ values for the TXT, SSC, SSC$\rho_b$ and the SSC$\rho_b$ + $\theta_{33}$ models were generally the lowest for the sandy loam and sandy clay loam classes (Table 5). Notice that the $RMSR_{wrc}$ for the clay loam class showed a significant improvement from the SSC$\rho_b$ to the SSC$\rho_b$ + $\theta_{33}$ model, whereas the $RMSR_{wrc}$ for the sand class decreased little even when $\theta_{33}$ was included. For this class much of the information about the particle-size distribution is lost in the sand fraction. The prediction of retention parameters for sandy soils probably could be improved if more fractions within the sand particle-size class were available (Vereecken et al., 1989; Schaap and Bouten, 1996).

A direct comparison of the hierarchical models and published PTFs is not easy. First, the published PTFs were calibrated on different data sets with possibly different distributions of data. Formally, we can only evaluate how well they perform on our, independent, data set. But if we assume that our data set is a fairly good representation of soils in the USA (cf., Fig. 1a and 1b), some degree of comparison is still possible, especially because we used the bootstrap to evaluate our neural networks on independent data. A second reason that complicates comparison is that neural networks and published PTFs use somewhat different input data. By approximation, the input data for function R3 (Cosby

**Table 5. Root mean square residuals for water retention data ($RMSR_{wrc}$) obtained on $N_{test}$ samples with four hierarchical models and four published pedotransfer functions (PTFs) for nine textural classes.**

| Class | Hierarchical models | | | | | Published PTFs† | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | TXT | SSC | SSC$\rho_b$ | SSC$\rho_b\theta_{33}$ | $N_{test}$ | R1 | R2 | R3 | R4 | $N_{test}$ |
| | $m^3\ m^{-3}$ | | | | | $m^3\ m^{-3}$ | | | | |
| Sand | 0.096 | 0.092 | 0.092 | 0.080 | 36 | 0.104 | 0.107 | 0.113 | 0.087 | 99 |
| Loamy sand | 0.102 | 0.107 | 0.100 | 0.054 | 49 | 0.114 | 0.126 | 0.112 | 0.091 | 136 |
| Sandy loam | 0.102 | 0.095 | 0.072 | 0.050 | 124 | 0.091 | 0.115 | 0.097 | 0.089 | 335 |
| Loam | 0.105 | 0.100 | 0.081 | 0.057 | 52 | 0.086 | 0.097 | 0.104 | 0.086 | 135 |
| Silts‡ | 0.123 | 0.124 | 0.096 | 0.071 | 82 | 0.114 | 0.105 | 0.134 | 0.111 | 218 |
| Sandy clay loam | 0.095 | 0.096 | 0.078 | 0.052 | 38 | 0.084 | 0.195 | 0.090 | 0.071 | 106 |
| Clay loam | 0.112 | 0.101 | 0.096 | 0.050 | 28 | 0.109 | 0.145 | 0.120 | 0.130 | 78 |
| Silty clay loam | 0.105 | 0.107 | 0.106 | 0.065 | 17 | 0.099 | 0.132 | 0.126 | 0.112 | 47 |
| Clays§ | 0.105 | 0.110 | 0.094 | 0.073 | 20 | 0.109 | 0.159 | 0.112 | 0.136 | 56 |
| Data set average | 0.107 | 0.104 | 0.087 | 0.060 | | 0.101 | 0.126 | 0.111 | 0.098 | |

† R1–R4: published water retention PTFs, see Table 1 for references. PTF R3 uses approximately the same input as the SSC neural network model while PTFs R1, R2, and R4 are comparable with the SSC$\rho_b$ model. Underlined values denote cases where the published PTFs provide better predictions than corresponding neural networks.
‡ Silt and silty loam.
§ Clay, silty clay, and sandy clay.

et al., 1984) model is comparable to the SSC model while the input data for R1 and R2 (Rawls and Brakensiek, 1985) models and R4 (Vereecken et al., 1989) are similar to the SSC$\rho_b$ model. The TXT and SSC$\rho_b$ + $\theta_{33}$ models do not have published PTFs with corresponding input data.

Based on average $RMSR_{wrc}$ values (bottom of Table 5), the hierarchical neural network models provided better estimates than the published PTFs by about 0.01 to 0.02 $m^3\ m^{-3}$ for the SSC and SSC$\rho_b$ models. The results in Table 5 also show that, because of an additional transformation step in its derivation (cf., Table 3), function R2 of Rawls and Brakensiek (1985) did not predict van Genuchten (1980) parameters as well as function R1 predicted the Brooks and Corey (1964) parameters. Coincidentally, function R2 was used by Carsel and Parrish (1988) to calculate class-average van Genuchten (1980) parameters. A few (underlined) cases are shown in Table 5 where the previously published PTFs provided better estimates than corresponding hierarchical neural network models. For example, function R1 predicted water retention slightly better for the silty clay loam class than the comparable SSC$\rho_b$ neural network model. Function R4 was somewhat better for the sand, loamy sand, and sandy clay loam classes. Following Tietje and Tapkenhinrichs (1993) and Kern (1995), we note that the function R4 (Vereecken et al., 1989) performed relatively well in comparison with other published PTFs. However, the neural network models yield better results for our data set, both on average and for most textural classes.

Table 6 shows similar results for $\log(K_s)$ predicted with four hierarchical neural network models and six published PTFs (K1–K6; Table 1). With respect to input data use, function K1 (Cosby et al., 1984) is comparable to the SSC model, while functions K2 (Brakensiek et al., 1984), K3 (Saxton et al., 1986), and K4 (Vereecken et al., 1990) are similar to the SSC$\rho_b$ model. The PTFs K5 (Ahuja et al., 1989) and K6 (Mishra and Parker, 1992) are comparable to the models using $EP_{33}$ and the $\theta_r\theta_s\alpha n$, respectively (Table 4).

The results in Table 6 indicate that, for most textural classes, the $RMSR_{Ks}$ decreased by about 0.2 log(cm $d^{-1}$) from the TXT models to the SSC$\rho_b$ + $\theta_{33}$ model. The RMSR of the sandy clay loam, clays, and clay loam classes showed less pronounced decreases. All previously published PTFs had higher RMSRs and lower $R^2$ than the neural network models. In terms of average $RMSR_{Ks}$, the best published PTF for predicting $K_s$ was K1 (Cosby et al., 1984). In terms of $R^2$, the best published

**Table 6. Root mean square residuals for data including saturated hydraulic conductivity ($RMSR_{Ks}$) obtained for $N_{test}$ samples for four hierarchical models and six published saturated hydraulic conductivity pedotransfer functions (PTFs).**

| Class | Hierarchical models | | | | | Published PTFs† | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | TXT | SSC | SSC$\rho_b$ | SSC$\rho_b\theta_{33}$ | $N_{test}$ | K1 | K2 | K3 | K4 | K5 | K6 | $N_{test}$ |
| | log (cm $d^{-1}$) | | | | | log (cm $d^{-1}$) | | | | | | |
| Sand | 0.510 | 0.433 | 0.408 | 0.319 | 36 | 0.613 | 0.519 | 0.421 | 0.883 | 0.362 | 0.525 | 97 |
| Loamy sand | 0.622 | 0.620 | 0.604 | 0.416 | 45 | 0.666 | 0.877 | 0.670 | 1.090 | 0.511 | 1.208 | 117 |
| Sandy loam | 0.652 | 0.638 | 0.521 | 0.466 | 74 | 0.795 | 0.777 | 0.625 | 0.815 | 0.627 | 1.615 | 199 |
| Loam | 0.643 | 0.667 | 0.488 | 0.470 | 12 | 0.860 | 0.530 | 0.611 | 0.587 | 0.847 | 1.317 | 32 |
| Silts‡ | 0.546 | 0.487 | 0.369 | 0.372 | 23 | 0.550 | 0.569 | 0.462 | 0.862 | 1.153 | 0.891 | 62 |
| Sandy clay loam | 0.724 | 0.711 | 0.668 | 0.598 | 30 | 0.957 | 0.868 | 1.344 | 1.178 | 1.155 | 1.660 | 80 |
| Clay loam | 0.684 | 0.642 | 0.573 | 0.586 | 2 | 0.980 | 0.624 | 0.630 | 0.678 | 0.790 | 0.726 | 6 |
| Silty clay loam | 0.637 | 0.468 | 0.423 | 0.363 | 3 | 0.624 | 1.003 | 0.526 | 0.960 | 1.852 | 0.749 | 10 |
| Clays§ | 0.491 | 0.453 | 0.506 | 0.459 | 6 | 0.545 | 1.704 | 1.441 | 0.914 | 0.674 | 1.707 | 17 |
| Dataset average | 0.627 | 0.602 | 0.533 | 0.451 | | 0.746 | 0.791 | 0.761 | 0.934 | 0.822 | 1.332 | |
| $R^2$ | 0.42 | 0.47 | 0.57 | 0.70 | | 0.30 | 0.42 | 0.43 | 0.22 | 0.54 | 0.21 | |

† K1–K6: published saturated hydraulic conductivity PTFs, see Table 2 for references. PTF K1 is approximately comparable to the SSC neural network model. PTFs K2, K3, and K4 are comparable to the SSC$\rho_b$ model. K5 and K6 are comparable to the EP33 and $\theta_r\theta_s\alpha n$ models in Table 4, respectively.
‡ Silt and silty loam.
§ Clay, silty clay, and sandy clay.

PTF was K5 (Ahuja et al., 1989). The overall $R^2$ for this PTF was 0.54, which is lower than the $R^2$ values of 0.65 and 0.67 obtained for the $EP_{10}$ and $EP_{33}$ neural network models (Table 4). The low $R^2$ in Table 6 for K4 was consistent with the low calibration $R^2$ listed in Table 2. The results for the PTFs of Cosby et al. (1984) and Saxton et al. (1986) were not as good as those reported by the researchers (0.839 and 0.95, respectively; cf., Table 2). Finally, we note that K6 performed relatively poorly, with an $RMSR_{Ks}$ that exceeded one order of magnitude.

## CONCLUSIONS

In this study we used a hierarchical neural network approach to predict hydraulic parameters. The basis of the analysis was a data set of 1209 samples, of which, horizon, sand, silt, and clay content, bulk density, porosity, and six to 13 retention points were known. A total of 620 samples also had measured $K_s$ data. We tested 12 different configurations of input data to predict water retention parameters of van Genuchten (1980), and we tried 19 different input configurations to predict $K_s$. The results show that $\theta_r$ was difficult to predict: $R^2$ never exceeded 0.41, even with the most relevant input. The correlation for the other parameters [$\theta_s$, log($\alpha$), log($n$), and log($K_s$)] increased from relatively low levels for an input configuration that used only textural classes, to about 0.70 for configurations that used sand, silt, and clay contents, bulk density, and one or two water content points. Root mean square residual water contents decreased from 0.107 $m^3 m^{-3}$ for a model that used only information about the soil textural class, to about 0.058 $m^3 m^{-3}$ for the best neural network model. However, even with the addition of a measured water content to the input, the $RMSR_{wrc}$ always stayed well above the $RMSR_{wrc}$ obtained for direct fits ($\approx$0.020 $m^3 m^{-3}$). Measured water retention curves appear to contain information that cannot be predicted from macroscopic variables like sand, silt, and clay contents, bulk density, and water retention. The $RMSR_{Ks}$ results decreased from about 0.627 log(cm $d^{-1}$) for a model that used only information about the soil textural class, to about 0.450 log(cm $d^{-1}$) for the best neural network models.

Uncertainty estimates for the predicted hydraulic properties were generated by combining the hierarchical models with the bootstrap method. Results of this approach showed that there can be a considerable uncertainty in predicted hydraulic properties. These uncertainties can be used in conjunction with the Richards equation to generate uncertainty estimates in simulated unsaturated flow processes.

Four selected neural network models were found to be better than four previously published PTFs for water retention parameters. Only the PTF of Vereecken et al. (1989) performed nearly as good as the neural network model with similar input requirements. None of the investigated existing PTFs for $K_s$ were found to be better than our neural network models.

We think that using the models from our hierarchical approach is not only attractive because of improved accuracy, but also because a neural network model can be chosen to match a particular availability of data. Because all neural network models were calibrated on the same data set, predictions of different models will be consistent. A final note may be that the neural network models are probably somewhat more difficult to implement than more traditional regression models. However, because the neural networks used in this study are basically simple matrix–vector operations, these limitations can be overcome. Currently, work is underway to implement some of the neural network models in user-friendly software.

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