Scaling Soil Water Retention Curves using a Correlation Coefficient Maximization Approach

LAKSHMAN NANDAGIRI

Department of Applied Mechanics and Hydraulics, National Institute of Technology Karnataka, Surathkal, India

JAN DE LEEUW

Department of Statistics, University of California, Los Angeles

In contrast to existing similar-media scaling methods which minimize sum of squared differences (SS) between a mean soil water retention curve and scaled soil water pressure data, we propose a new method involving maximization of the correlation coefficient (R) between measured and estimated soil water pressure heads. With this new criterion, multivariate statistical procedures are implemented resulting in an explicit non-iterative solution for the set of scale factors describing the spatial variability of measured soil water retention curves. Performance of the proposed method was tested with published data of in-situ soil water retention measurements made at a site in North Dakota, USA. Scaling was successful as indicated by substantial reduction in SS and matched reported performances of existing iterative methods. For the dataset used, our algorithm provides the optimal solution in a non-iterative manner and introduces minimal distortions into original retention measurements.

INTRODUCTION

Regression-based functional normalization techniques (Tillotson and Neilsen, 1984) are simple scaling tools that may be used to characterize and quantify spatial variability of soil hydraulic properties. By providing information on the structure of spatial heterogeneity in soil water retention and hydraulic conductivity curves, scaling facilitates stochastic
simulation of soil water/solute flow at field and watershed scales (e.g., Peck et al., 1977; Sharma and Luxmoore, 1979; Hopmans and Stricker, 1989; Ünlü et al., 1990).

Scaling methods use measured data sets of soil water pressure ($h$) versus soil moisture content ($\theta$) and hydraulic conductivity ($K$) versus $\theta$ (or $h$) obtained from a number of locations in a heterogeneous landscape and yield two sets of scale factors ($\alpha$) relating the soil water retention curve [$h(\theta)$] and the hydraulic conductivity curve [$K(\theta)$ or $K(h)$] at each location to their respective representative mean curves.

Although similitude requirements demand that the scale factor derived at a sampling location from the $h(\theta)$ curve be identical to that derived from the $K(\theta)$ curve, field soils rarely appear to behave as perfect similar media. To counter this, Clausnitzer et al. (1992) proposed a novel method of scaling both curves simultaneously to yield a single set of scale factors. Nevertheless, most earlier investigators have observed: i) high degree of correlation between the two sets of scale factors for a wide variety of soils (Warrick et al., 1977; Russo and Bresler, 1980) ii) more effective scaling of $K(\theta)$ curves using scale factors derived from $h(\theta)$ curves (Warrick et al., 1977) and iii) negligible errors in simulating soil water processes using scale factors derived from $h(\theta)$ data alone (Ahuja et al., 1984). Consequently, based on the assumption of approximate similar-media behavior, it is generally accepted that a single set of scale factors derived from scaling soil water retention data alone may be sufficient to describe the spatial variability of both hydraulic functions (Hopmans and Stricker, 1989).

Several similar-media methods (under the class of functional normalization techniques) to scale soil water retention curves have been proposed (e.g., Warrick et al., 1977; Russo and Bresler, 1980; Rao et al., 1983; Ahuja et al., 1984; Williams and Ahuja, 1992; Daamen et al., 1991; Clausnitzer et al., 1992), but all of them are based on determining optimal scale factors through some form of minimization of the sum of squared differences (SS) between a mean curve and scaled water retention data. As Hopmans (1987) notes in a
comparative evaluation of several approaches, methods differ mostly in the manner in which the mean $h(\theta)$ curve is represented.

In this technical note, we present a new method to scale soil water retention curves through maximization of the correlation coefficient ($R$) between soil water pressure heads estimated from a mean curve and measured pressure heads. Although one may prove from statistical theory that maximizing $R$ is equivalent to minimizing $SS$, we felt it was worthwhile investigating the former approach with the objective of being able to take advantage of analogous procedures adopted in multivariate statistical methods, notably canonical correlation. Accordingly, our algorithm yields an explicit non-iterative solution for the optimal scale factors and constitutes an improvement over existing methods, which employ iterative solution procedures.

In subsequent sections of this note, we present the theory of regression-based similar-media scaling and a description of the proposed $R$-maximization scaling procedure, and demonstrate its application using a dataset of soil water retention measurements made by earlier investigators in North Dakota, USA.

THEORY

*Similar-Media Scaling*

Scaling theory, based on the concept of similar media assumes that, if $(h, \theta)$ are measured values of soil water pressure (negative in unsaturated soils but treated as positive in this paper) and corresponding soil moisture content at any location, then $h$ is related to a mean soil water pressure ($\hat{h}$) corresponding to the same moisture content through the scaling relationship,
\[ h = \left( \frac{\tilde{\lambda}}{\lambda} \right) \frac{\tilde{h}}{\alpha} \]  

(1)

where \( \tilde{\lambda} \) and \( \lambda \) represent microscopic characteristic lengths of the reference soil and the soil at the particular location respectively, and \( \alpha \) is the scale factor which is constant for the location for all values of moisture contents. However, owing to differences in pore structures of soils, use of effective saturation \( \Theta = (\theta - \theta_r)/(\theta_s - \theta_r) \) (where subscripts \( s \) and \( r \) refer to saturation and residual moisture contents respectively), is preferred to the use of \( \theta \). The objective of all scaling methods is to derive values of \( \alpha \), one for each sampling location, and thereby characterize the spatial variability in \( h(\Theta) \) curves.

An attractive choice for representing the soil water retention curve is the model proposed by van Genuchten (1980):

\[ \Theta = \left[ 1 + \left( \frac{\gamma h}{\Theta^{\frac{1}{n}} - 1} \right)^n \right]^{-\frac{n-1}{n}} \]  

(2)

which may be re-cast as,

\[ \hat{h} = \left[ \left( \frac{\theta_s}{\Theta^{\frac{1}{n}} - 1} \right)^{\frac{n}{n-1}} \right]^{-1} \]  

(3)

in which and \( \gamma \) and \( n \) are fitting parameters.

As a first step, Equation (3) is fitted to \((h, \theta)\) observations made at each location and optimal values of \( \theta_s \) and \( \theta_r \) obtained are used to transform observed \( \theta \) values at each location
to corresponding \( \Theta \) values. Equation (3) is then fitted to \((h, \Theta)\) observations pooled from all sampling locations so as to derive optimal values of model parameters \( \gamma \) and \( n \). The optimized form of Equation (3) is then representative of the first estimate of the mean soil water retention curve for all the sampled locations.

Assuming that the similar media scaling relationship [Equation (1)] is valid for all \( h \) values at all locations, a set of scale factors may be derived by minimization of the sum of squared differences (SS) between the mean curve and scaled data.

\[
\text{SS} = \sum_{j=1}^{M} \left( \sum_{i=1}^{n_j} \left( h_{ij} - \alpha_j \hat{h}_{ij} \right)^2 \right) \text{ for } i=1\ldots n_j; j=1,\ldots,M
\]

(4)

where \( h_{ij} \) is the \( i \)th soil water pressure head measured at the \( j \)th location, \( \hat{h}_{ij} \) is the \( i \)th mean soil water pressure head at the \( j \)th location, \( n_j \) is the number of observations at the \( j \)th location and \( M \) is the total number of sampled locations.

Analytical procedures for minimization of SS may then be employed by setting,

\[
\frac{\partial (\text{SS})}{\partial \alpha_j} = 0 \quad j=1,\ldots,M
\]

(5)

subject to a normalizing constraint

\[
\sum_{j=1}^{M} \alpha_j = M
\]

(6)

This procedure yields the desired solution of the set of scale factors, [for example, refer Equations (19) and (20) of Clausnitzer et. al., 1992]. However, optimal scale factors
still need to be determined through an iterative process in which Equation (3) is fitted to
scaled soil water pressures using scale factors obtained in the previous iteration. The
procedure is repeated until SS converges to a minimum or if convergence is not obtained, the
smallest SS attained is assumed to yield the optimal set of scale factors.

Proposed R-maximization Scaling Procedure

Instead of defining SS [Equation (4)] and minimizing it using Equations (5) and (6),
we work with the correlation coefficient (R) between the two variables \( \hat{h} \) and \( h \), defined in
general terms as:

\[
R(\hat{h}, h) = \frac{\text{cov}(\hat{h}, h)}{\sqrt{\text{var}(h) \cdot \text{var}(\hat{h})}}
\]

For convenience, we use matrix notations and accordingly define \( \mathbf{h} \) to be a \((n \times 1)\) vector containing \( n \) observations of soil water pressure heads and \( \hat{\mathbf{h}} \) to be a \((n \times 1)\) vector of \( n \) estimates of water pressure heads, both corresponding to the same values of effective
saturation \( \Theta \). The \( n \) values are partitioned into \( M \) groups (corresponding to sampling
locations) each with \( n_j \) values such that \( \sum_{j=1}^{M} n_j = n \). We set \( k_j = n_j / n \).

Let \( h_j \) and \( u_j \) represent the group means and group variances of \( h \), and \( \hat{h}_j \) and \( v_j \) the
corresponding group means and group variances of \( \hat{h} \). Let \( c_j \) represent the group covariances
between \( h \) and \( \hat{h} \).

The total covariance for the \( n \) observations of \( h \) and \( \hat{h} \) may be written as,
\[
\text{cov}(\hat{h}, h) = \sum_{j=1}^{M} k_j c_j + \left\{ \sum_{j=1}^{M} k_j h_j \hat{h}_j - \left( \sum_{j=1}^{M} k_j h_j \right) \right\}
\]  

(8)

and the total variance of \( h \) will be,

\[
\text{var}(h) = \sum_{j=1}^{M} k_j u_j + \left\{ \sum_{j=1}^{M} k_j h_j^2 - \left( \sum_{j=1}^{M} k_j h_j \right)^2 \right\}
\]  

(9)

Now, if all values of \( h \) in group \( j \) are multiplied by a weight \( \beta_j \), the total covariance and variance get modified as,

\[
\text{cov}(\hat{h}, \beta h) = \sum_{j=1}^{M} k_j \beta_j c_j + \left\{ \sum_{j=1}^{M} k_j \beta_j h_j \hat{h}_j - \left( \sum_{j=1}^{M} k_j \beta_j h_j \right) \right\}
\]  

(10)

\[
\text{var}(\beta h) = \sum_{j=1}^{M} k_j \beta_j^2 u_j + \left\{ \sum_{j=1}^{M} k_j \beta_j^2 h_j^2 - \left( \sum_{j=1}^{M} k_j \beta_j h_j \right)^2 \right\}
\]  

(11)

The total variance [Equation (10)] may be represented in matrix form as,

\[
\text{cov}(\hat{h}, \beta h) = g' \beta
\]  

(12)

where \( g' \) is the transpose of a \((M \times 1)\) vector \( g \) whose elements are given by,
\[ g_j = k_j \left\{ c_j + h_j \left( h_j - \sum_{j=1}^{M} k_j h_j \right) \right\} \quad \text{for } j = 1, \ldots, M \]  

Similarly, total variance [Equation (11)] may be written as,

\[ \text{var}(\beta h) = \beta' A \beta \]  

where \( A \) is a \((M \times M)\) symmetric matrix whose diagonal elements are defined by,

\[ a_{jj} = k_j \left( u_j + h_j^2 - k_j h_j^2 \right) \quad \text{for } j = q \]  

and off-diagonal elements by,

\[ a_{jq} = -k_j h_j k_q h_q \quad \text{for } j \neq q \]

with \( j = 1, \ldots, M \) and \( q = 1, \ldots, M \)

Using Equation (7) we may now write the correlation coefficient as a function of weights \( \beta \) as,

\[ R(\hat{h}, \beta h) = \frac{\text{cov}(\hat{h}, \beta h)}{\sqrt{\text{var}(\beta h)\text{var}(\hat{h})}} = \frac{g' \beta}{\left\{ \beta' A \beta \right\}^{1/2} \left\{ \text{var}(\hat{h}) \right\}^{1/2}} \]
The objective is to determine the \((M \times 1)\) vector \(\beta\) that maximizes \(R(\hat{h}, \beta h)\). To ensure a unique solution, it is necessary to constrain \(\text{var}(\beta h)\) in Equation (17) to unity while maximizing \(\text{cov}(\hat{h}, \beta h)\) [Morrison, 1990]. Note that \(\text{var}(\hat{h})\) is constant and remains unaffected by \(\beta\).

Accordingly, we set up the maximization problem,

\[
\frac{\partial R(\hat{h}, \beta h)}{\partial \beta} = 0
\]  \hspace{1cm} (18)

subject to the constraint,

\[
\beta' A \beta = 1
\]  \hspace{1cm} (19)

Introducing the Lagrangian multiplier \((\mu)\), the optimization problem defined by Equation (18) reduces to,

\[
g - \mu A \beta = 0
\]  \hspace{1cm} (20)

From Equation (20) we have,

\[
\beta = \frac{1}{\mu} A^{-1} g
\]  \hspace{1cm} (21)

which upon substitution into the constraint defined by Equation (19) yields,
\[ \mathbf{\beta}' \mathbf{A} \mathbf{\beta} = \frac{1}{\mu^2} \mathbf{g}' \mathbf{A}^{-1} \mathbf{g} = 1 \]  

This implies,

\[ \mu = \sqrt{\mathbf{g}' \mathbf{A}^{-1} \mathbf{g}} \]  

Combining Equations (21) and (23), we get the expression of the desired optimal (M x 1) vector \( \mathbf{\beta} \) that maximizes the correlation coefficient as,

\[ \mathbf{\beta} = \frac{\mathbf{A}^{-1} \mathbf{g}}{\sqrt{\mathbf{g}' \mathbf{A}^{-1} \mathbf{g}}} \]  

and the optimal correlation coefficient as,

\[ R = \frac{\sqrt{\mathbf{g}' \mathbf{A}^{-1} \mathbf{g}}}{\sqrt{\text{var}(h)}} \]  

Any scalar operation on \( \mathbf{\beta} \) will not change its optimality property. Hence, we apply the normalizing constraint given by Equation (6) through the following operation [Equation (26)] to ensure that our vector of weights \( \mathbf{\beta} \) is comparable to scale factors \( \mathbf{\alpha} \) derived by other investigators.
The following steps may be adopted for implementing the proposed method.

1. For each group (location) determine $k_j, \hat{h}_j, h_j, u_j, \text{ and } c_j$.

2. Use Equation (13) to setup the $\mathbf{g}$ vector and Equations (15) & (16) to setup the $\mathbf{A}$ matrix.

3. Compute $\mathbf{g}'$ and $\mathbf{A}^{-1}$.

4. Determine the optimal vector of weights $\mathbf{b}$ using Equation (24) and the optimal correlation coefficient using Equation (25).

5. Transform $\mathbf{b}$ into equivalent vector of scale factors $\mathbf{a}$ using Equation (26).

EXAMPLE APPLICATION

To demonstrate the applicability of the proposed R-maximization procedure for scaling water retention curves, we used measurements made by Schuh et al., (1991) in Dickey County, North Dakota, USA. Their dataset comprises in-situ soil water retention measurements made using a paired neutron probe-tensiometers setup during profile internal drainage tests at a number of sites. For this study, we selected water retention data $(h, \theta)$ of the \text{Ap} horizon (8 cm depth) at five sites (A, B, C, D, E) located in two topo-sequences separated by a distance of 8 km. In all, measurements pooled from the five locations yielded 130 data points, which we felt was sufficient to demonstrate our procedure.

Computations were performed in Microsoft Excel®, spreadsheet software. We used the Solver Add-in® to fit Equation (3) to retention data as per the methodology suggested by Wraith and Or (1998) and a freeware add-in (Matrix 1.3) to perform matrix operations.

The performance of the scaling method was evaluated using the following criteria:
i) percentage reduction in SS [Equation (4)] prior to and after scaling ii) correlation coefficient ($R_{US-DS}$) between unscaled $h$ data and descaled $h$ data obtained by applying the appropriate scale factor to the final mean soil water retention curve and iii) root mean square error ($RMSE$) between unscaled and descaled $h$ data.

RESULTS AND DISCUSSION

Figure 1 shows the effect of scaling on measured soil water retention data. Unscaled $h$ values which are scattered around a mean soil water retention curve, coalesce into a narrow band around the final curve. Table 1 shows the set of optimal scale factors that bring about this transformation and Table 2 shows van Genuchten model parameters of the mean soil water retention curve prior to and after scaling.

Performance criteria for the scaling method are summarized in Table 3. Starting with a large SS of 51926 and a correlation coefficient (R) of 0.698 between unscaled $h$ data and $\hat{h}$ values, our algorithm attains the maximum possible value of $R = 0.9589$. SS reduces to 3060 indicating an impressive reduction of 90.6%. Although we implemented an iterative procedure in an effort to further maximize R, the result obtained at the end of the first iteration [Table 3] was the optimal one. In comparison, Warrick et. al., (1977) report SS reduction of 54.5% at the end of the first iteration and maximum reduction of 85.5% after 10 iterations, when applying a SS-minimization scaling method to retention data of a Panoche soil. Using a similar SS-minimization method to scale water retention data of a sandy loam soil, Clausnitzer et. al., (1992) report SS reductions of 95.5% and 83.1% for A and B soil horizons respectively, but the number of iterations employed is not reported. Our optimal solution also appears to introduce small distortions into the original $h$ data as indicated by $R_{US-DS}$ of 0.8742 and RMSE of 14.23 cm, results which are similar to those reported for existing SS-minimization methods (Hopmans, 1987). Figure 2 provides a graphical comparison of original measurements and descaled values of $h$. 
CONCLUSIONS

While existing scaling methods are based on minimization of sum of squared differences (SS) between a mean soil water retention curve and scaled hydraulic data, we propose a new algorithm based on maximization of correlation coefficient (R) between measured and estimated soil water pressure heads. Preliminary tests indicated satisfactory performance of the proposed method when applied to in-situ measured soil water retention measurements. For the data set used, the algorithm yields the optimal solution in a non-iterative manner. However, more comprehensive evaluation with larger and more diverse data sets is needed to validate these findings and also to determine the probability distribution of scale factors derived using the proposed method. Since similar-media scaling techniques are nowadays being incorporated into hydrologic models, an example being the Root Zone Water Quality Model (RZWQM) (Starks et. al., 2003), a non-iterative method of the type proposed in this work would be more amenable for integration into such modeling systems.

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REFERENCES


Wraith, J.M., and Dani Or, Nonlinear parameter estimation using spreadsheet software. J.

FIGURE CAPTIONS

Figure 1: a) Original and b) scaled soil water retention data and fitted mean curves

Figure 2: Comparison of original and descaled soil water pressure head
TABLE 1: Optimal Scale Factors

<table>
<thead>
<tr>
<th>Site</th>
<th>$\alpha$</th>
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<tbody>
<tr>
<td>A</td>
<td>1.3828047</td>
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<tr>
<td>B</td>
<td>1.2753658</td>
</tr>
<tr>
<td>C</td>
<td>0.7724469</td>
</tr>
<tr>
<td>D</td>
<td>0.6986128</td>
</tr>
<tr>
<td>E</td>
<td>0.8707697</td>
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TABLE 2: Van Genuchten Model [Equation (3)] parameters for mean soil water retention curve

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unscaled</th>
<th>Scaled</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\gamma$ (cm$^{-1}$)</td>
<td>0.014616</td>
<td>0.016312</td>
</tr>
<tr>
<td>$n$</td>
<td>6.101295</td>
<td>4.485661</td>
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</table>

TABLE 3: Performance Criteria for Proposed Scaling Method

<table>
<thead>
<tr>
<th>Criteria</th>
<th>Unscaled</th>
<th>Scaled</th>
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</thead>
<tbody>
<tr>
<td>SS</td>
<td>51926</td>
<td>8196</td>
</tr>
<tr>
<td>%SS reduction</td>
<td>-</td>
<td>84.2</td>
</tr>
<tr>
<td>$R$</td>
<td>0.6980</td>
<td>0.9589</td>
</tr>
<tr>
<td>$R_{US-DS}$</td>
<td>-</td>
<td>0.8742</td>
</tr>
<tr>
<td>RMSE</td>
<td></td>
<td>14.23</td>
</tr>
</tbody>
</table>
Fig. 1. a) Original and b) scaled soil water retention data and fitted mean curves
Fig. 2. Comparison of original and descaled soil water pressure head