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 (eg., Peck et al, 1977; Sharma and Luxmoore, 1979; Hopmans and Stricker, 1989; Űnlu et.al., 1990).

Scaling methods use measured data sets of soil water pressure (*h*) versus soil moisture content (θ) and hydraulic conductivity (*K*) versus θ (or *h*) obtained from a number of locations in a heterogeneous landscape and yield two sets of scale factors (α) 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, θ) 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,

$$h = \left(\frac{\bar{\lambda}}{\lambda} \right) \hat{h} = \frac{\hat{h}}{\alpha} \quad (1)$$

where $\bar{\lambda}$ and λ represent microscopic characteristic lengths of the reference soil and the soil at the particular location respectively, and α 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 θ. The objective of all scaling methods is to derive values of α, 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):

$$\Theta = \left[1 + \left(\gamma \hat{h} \right)^{n} \right]^{-\left(\frac{n-1}{n}\right)} \quad (2)$$

which may be re-cast as,

$$\hat{h} = \left[\left(\Theta^{-\frac{n}{n-1}} - 1 \right)^{\frac{1}{n}} \right] \gamma^{-1} \quad (3)$$

in which and γ and *n* are fitting parameters.

As a first step, Equation (3) is fitted to (h,θ) observations made at each location and optimal values of θ_s and θ_r obtained are used to transform observed θ values at each location to corresponding Θ values. Equation (3) is then fitted to (h,Θ) observations pooled from all sampling locations so as to derive optimal values of model parameters γ 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.

$$SS = \sum_{j=1}^{M} \sum_{i=1}^{n_j} \left(\hat{h}_{i,j} - \alpha_j h_{i,j} \right)^2 \quad \text{for } i=1\ldots n_j;\ j=1,\ldots..M \qquad (4)$$

where $h_{i,j}$ is the i[th] soil water pressure head measured at the j[th] location, $\hat{h}_{i,j}$ 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,

$$\frac{\partial (SS)}{\partial \alpha_j} = 0 \qquad j=1,\ldots\ldots M \qquad (5)$$

subject to a normalizing constraint

$$\sum_{j=1}^{M} \alpha_j = M \qquad (6)$$

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:

$$\mathrm{R}\left(\hat{\mathrm{h}}, \mathrm{h}\right) = \frac{\mathrm{cov}\left(\hat{\mathrm{h}}, \mathrm{h}\right)}{\sqrt{\mathrm{var}(\hat{\mathrm{h}})\ \mathrm{var}(\mathrm{h})}} \tag{7}$$

For convenience, we use matrix notations and accordingly define $\mathbf{h}$ to be a (n x 1) vector containing n observations of soil water pressure heads and $\hat{\mathbf{h}}$ to be a (n x 1) vector of n estimates of water pressure heads, both corresponding to the same values of effective saturation Θ. 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,

$$\operatorname{cov}\left(\hat{h}, h\right) = \sum_{j=1}^{M} k_j c_j + \left\{ \sum_{j=1}^{M} k_j h_j \hat{h}_j - \sum_{j=1}^{M} k_j h_j \sum_{j=1}^{M} k_j \hat{h}_j \right\} \tag{8}$$

and the total variance of **h** will be,

$$\operatorname{var}(h) = \sum_{j=1}^{M} k_j u_j + \left\{ \sum_{j=1}^{M} k_j h_j^2 - \left(\sum_{j=1}^{M} k_j h_j \right)^2 \right\} \tag{9}$$

Now, if all values of *h* in group j are multiplied by a weight β_j, the total covariance and variance get modified as,

$$\operatorname{cov}\left(\hat{\mathrm{h}}, \beta \mathrm{h}\right) = \sum_{\mathrm{j}=1}^{\mathrm{M}} \mathrm{k}_{\mathrm{j}} \beta_{\mathrm{j}} \mathrm{c}_{\mathrm{j}} + \left\{ \sum_{\mathrm{j}=1}^{\mathrm{M}} \mathrm{k}_{\mathrm{j}} \beta_{\mathrm{j}} \mathrm{h}_{\mathrm{j}} \hat{\mathrm{h}}_{\mathrm{j}} \sum_{\mathrm{j}=1}^{\mathrm{M}} \mathrm{k}_{\mathrm{j}} \beta_{\mathrm{j}} \mathrm{h}_{\mathrm{j}} \sum_{\mathrm{j}=1}^{\mathrm{M}} \mathrm{k}_{\mathrm{j}} \hat{\mathrm{h}}_{\mathrm{j}} \right\} \tag{10}$$

$$\operatorname{var}(\beta h) = \sum_{j=1}^{M} k_j \beta_j^2 u_j + \left\{ \sum_{j=1}^{M} k_j \beta_j^2 h_j^2 - \left(\sum_{j=1}^{M} k_j \beta_j h_j \right)^2 \right\} \tag{11}$$

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

$$\operatorname{cov}\left(\hat{h}, \beta h\right) = \mathbf{g}' \boldsymbol{\beta} \tag{12}$$

where $\mathbf{g}'$ is the transpose of a (M x 1) vector $\mathbf{g}$ whose elements are given by,

$$\mathbf{g}_j = k_j\left\{c_j + h_j\left(\hat{h}_j - \sum_{j=1}^{M} k_j \hat{h}_j\right)\right\} \qquad \text{for j=1,}\ldots M \tag{13}$$

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

$$\operatorname{var}(\beta h) = \boldsymbol{\beta}'\mathbf{A}\,\boldsymbol{\beta} \tag{14}$$

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

$$a_{jq} = k_j\left(u_j + h_j^2 - k_j\, h_j^2\right) \qquad \text{for } j = q \tag{15}$$

and off-diagonal elements by,

$$a_{jq} = -\,k_j h_j k_q h_q \qquad \text{for } j \neq q \tag{16}$$

with j=1,….M and q = 1,….M

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

$$R\left(\hat{h}, \beta h\right) = \frac{\operatorname{cov}\left(\hat{h}, \beta h\right)}{\sqrt{\operatorname{var}(\beta h) Var(\hat{h})}} = \frac{\mathbf{g}'\,\boldsymbol{\beta}}{\left\{\boldsymbol{\beta}'\ \mathbf{A}\,\boldsymbol{\beta}\right\}^{1/2}\left\{Var\left(\hat{h}\right)\right\}^{1/2}} \tag{17}$$

The objective is to determine the (M x 1) vector $\boldsymbol{\beta}$ that maximizes $R(\hat{h}, \beta h)$. To ensure a unique solution, it is necessary to constrain var(βh) in Equation (17) to unity while maximizing cov($\hat{h}$, βh)[Morrison, 1990]. Note that var($\hat{h}$) is constant and remains unaffected by β.

Accordingly, we set up the maximization problem,

$$\frac{\partial R\left(\hat{h}, \beta h\right)}{\partial \beta} = 0 \tag{18}$$

subject to the constraint,

$$\boldsymbol{\beta}' \mathbf{A} \boldsymbol{\beta} = 1 \tag{19}$$

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

$$\mathbf{g} - \mu \mathbf{A} \boldsymbol{\beta} = 0 \tag{20}$$

From Equation (20) we have,

$$\boldsymbol{\beta} = \frac{1}{\mu} \mathbf{A}^{-1} \mathbf{g} \tag{21}$$

which upon substitution into the constraint defined by Equation (19) yields,

$$\boldsymbol{\beta}^{'}\mathbf{A}\boldsymbol{\beta} = \frac{1}{\mu^{2}}\mathbf{g}^{'}\mathbf{A}^{-1}\mathbf{g} = 1 \tag{22}$$

This implies,

$$\mu = \sqrt{\mathbf{g}^{'}\,\mathbf{A}^{-1}\,\mathbf{g}} \tag{23}$$

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

$$\boldsymbol{\beta} = \frac{\mathbf{A}^{-1}\mathbf{g}}{\sqrt{\mathbf{g}^{'}\,\mathbf{A}^{-1}\mathbf{g}}} \tag{24}$$

and the optimal correlation coefficient as,

$$R = \frac{\sqrt{\mathbf{g}^{'}\,\mathbf{A}^{-1}\,\mathbf{g}}}{\sqrt{\mathrm{var}\left(\hat{h}\right)}} \tag{25}$$

Any scalar operation on $\boldsymbol{\beta}$ 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 $\boldsymbol{\beta}$ is comparable to scale factors $\boldsymbol{\alpha}$ derived by other investigators.

$$\boldsymbol{\alpha} = \frac{\mathrm{M}}{\sum_{j=1}^{M} \beta_j} \boldsymbol{\beta} \tag{26}$$

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, 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 $\boldsymbol{\beta}$ using Equation (24) and the optimal correlation coefficient using Equation (25).
5. Transform $\boldsymbol{\beta}$ into equivalent vector of scale factors $\boldsymbol{\alpha}$ 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,θ) of the A_p 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 ($R_{US\text{-}DS}$) 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 $R_{US\text{-}DS}$ 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.

Acknowledgements. We thank William M. Schuh, North Dakota Water Commission, for providing soils data and Jan Hopmans, University of California, Davis for words of encouragement.

REFERENCES

Ahuja, L.R., J.W.Nancy, and D.R.Nielsen, Scaling soil water properties and infiltration modelling, *Soil Sci. Soc. Am.J.,* 48, 970-973, 1984.

Clausnitzer, V., J.W. Hopmans, and D.R.Nielsen, Simultaneous scaling of soil water retention and hydraulic conductivity curves, *Water Resour. Res.,* 28, 19-31, 1992.

Daamen, C.C., Zhenhua Xiao, and J.A.Robinson, Estimation of water retention function using scaling theory and soil physical properties, *Soil Sci. Soc. Am. J.,* 55, 8-13, 1991.

Hopmans, J.W., A comparison of various methods to scale soil hydraulic properties, *J. Hydrol.,* 93, 241-256, 1987.

Hopmans, J.W., and J.N.M.Stricker, Stochastic analysis of soil water regime in a watershed, *J. Hydrol.,* 105, 57-84, 1989.

Matrix 1.3, http://digilander.liberto.it/foxes/matrix13.zip

Morrison, D.F., Multivariate statistical methods, McGraw-Hill Inc., 495 p, 1990.

Peck, A.J., R.J. Luxmoore, and J.C. Stolzy, Effects of spatial variability of soil hydraulic properties in water budget modeling, *Water Resour. Res.,* 13, 348-354, 1977.

Rao, P.S.C., R.E. Jessup, A.C. Hornsby, D.K. Cassel, and W.A. Pollens, Scaling soil microhydrological properties of Lakeland and Konowa soils using similar media concepts, *Agric. Water Manage.,* 6, 277-290, 1983.

Russo, D., and E. Bresler, Scaling soil hydraulic properties of a heterogeneous field, *Soil Sci. Soc. Am. J.,* 44, 681-684, 1980.

Schuh, W.M., R.L. Cline and M.D. Sweeney, Unsaturated soil hydraulic properties and parameters for the Oakes area, Dickey County, North Dakota, Water Resources Investigation No.18, North Dakota State Water Commision, 1991.

Sharma, M.L., and R.J. Luxmoore, Soil spatial variability and its consequences on simulated water balance, *Water Resour. Res.,* 15, 1567-1573, 1979.

Starks, P.J., G.C. Heathman, L.R. Ahuja and Liwang Ma, Use of limited soil property data and modeling to estimate root zone soil water content. *J. Hydrol.,* 272, 131-147, 2003.

Tillotson, P.M., and D.R. Nielsen, Scale factors in soil science, *Soil Sci. Soc. Am.J.,* 48, 953-959, 1984.

Ünlu, K., D.R. Nielsen, and J.W. Biggar, Stochastic analysis of unsaturated flow: One-dimensional Monte Carlo simulations and comparisons with spectral perturbation analysis and field observations, *Water Resour. Res.,* 26, 2207-2218, 1990.

Van Genuchten, M.T., A closed form equation for predicting the hydraulic conductivity of unsaturated soils, *Soil Sci. Sco. Am. J.,* 44, 892-898, 1980.

Warrick, A.W., G.J. Mullen and D.R. Nielsen, Scaling field measured soil hydraulic properties using a similar media concept, *Water Resour. Res.,* 13, 355-362, 1977.

Williams, R.D., and L.R.Ahuja, Evaluation of similar-media scaling and a one-parameter model for estimating the soil water characteristic, *J. Soil Sci.,* 43, 237-248, 1992.

Wraith, J.M., and Dani Or, Nonlinear parameter estimation using spreadsheet software. *J. Nat. Resour. Life Sci. Educ.,* 27, 13-19, 1998.

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

Site	α
A	1.3828047
B	1.2753658
C	0.7724469
D	0.6986128
E	0.8707697

TABLE 2:Van Genuchten Model [Equation (3)] parameters for mean soil water retention curve

Parameter	Unscaled	Scaled
γ (cm^{-1})	0.014616	0.016312
n	6.101295	4.485661

TABLE 3: Performance Criteria for Proposed Scaling Method

Criteria	Unscaled	Scaled
SS	51926	8196
%SS reduction	-	84.2
R	0.6980	0.9589
$R_{US\text{-}DS}$	-	0.8742
RMSE		14.23

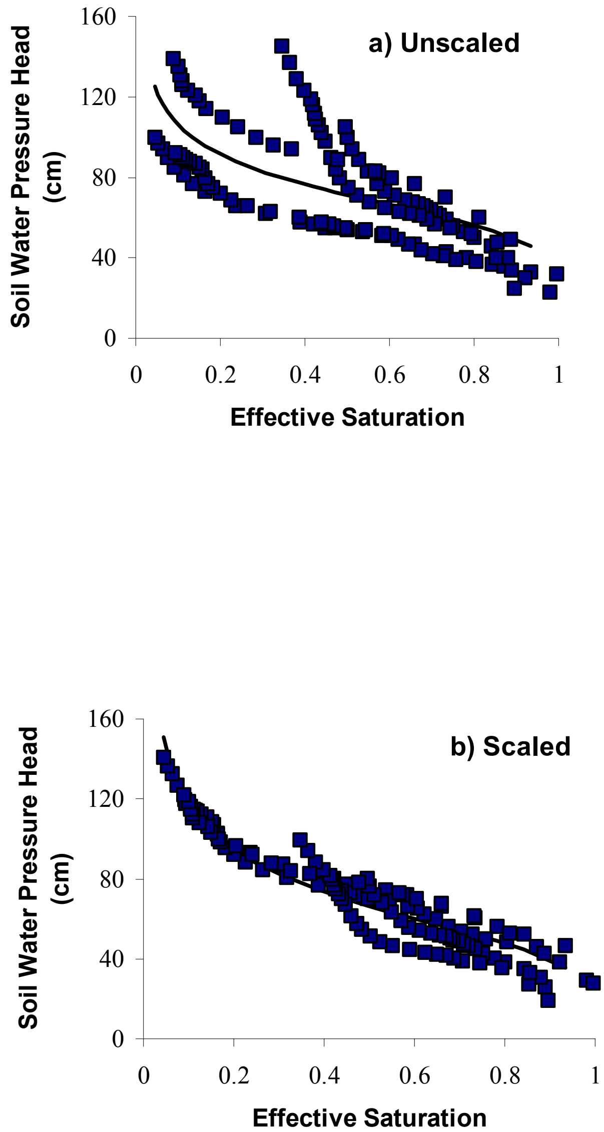

Fig. 1. a) Original and b) scaled soil water retention data and fitted mean curves

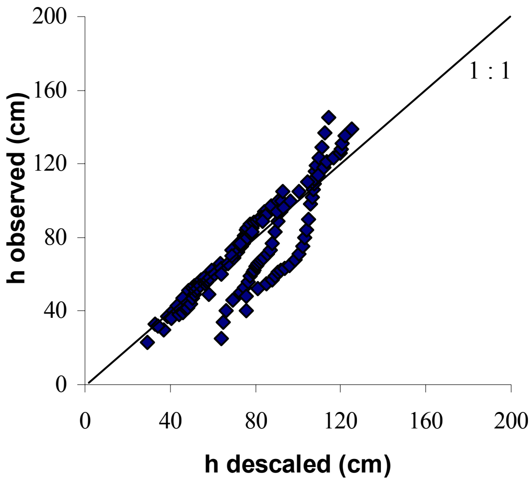

Fig. 2. Comparison of original and descaled soil water pressure head