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Research Paper

Estimating water retention characteristic parameters using differential evolution

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ABSTRACT

The water retention curve has a key role for the hydraulic characterization of porous media. A new method, based on the differential evolution algorithm, for the determination of the characteristic parameters of several water retention models from the experimental data is proposed. We present the details of the method and its application to the calculation of water retention curves of soils. We show that our method can find the optimal model parameters without any prior information on the characteristics of the medium under investigation. The errors associated to the calculated parameters are evaluated through the random perturbation of the data.

1. Introduction

The water retention curve (WRC) relates the amount of water contained in a porous medium to the adsorption and capillary forces holding it. This relationship is a key property for studying several hydraulic processes in soils or rocks, such as drainage, infiltration, solute diffusion, water flow, mass transport or recharge of aquifers.

The analytic form of the WRC is a nonlinear function $\theta(\psi)$ that describes the relation between the suction ψ and the volumetric water content θ. Several models have been developed to describe the shape of the WRC across the widest possible range of suction, such as the well known and widely used models of Brooks-Corey [1], van Genuchten [2] and Rossi-Nimmo [3].

These models depend on a set of parameters that are characteristic of the porous medium under investigation and whose values are determined by fitting the model equation to the experimental measurements. The best set of characteristic parameters is usually calculated using an optimization method based on nonlinear least-squares (NLS), that minimizes an objective function describing the difference between the measured data and those predicted by the model.

A serious drawback of NLS methods is that they do not guarantee to converge to the absolute (or global) minimum of the objective function. Depending on the initial estimate of the characteristic parameters, calculations may easily get stuck in one of the local minima instead of locating the global minimum of the objective function [4].

Heuristic global optimization methods, such as simulated annealing [5], genetic algorithm [6], ant colony optimization [7], particle swarm optimization [8], are better suited than NLS methods to locate the global minimum, without needing a "good" initial estimate of the model parameters. All these methods have been extensively used in soil science to calculate the hydraulic parameters of porous media [9–13]. However, as shown below, even these heuristic methods have serious shortcomings.

Differential evolution [14] is a versatile heuristic global optimization method particularly well suited to solve multidimensional optimization problems involving continuous variables [15]. To the best of our knowledge, differential evolution has not been applied yet to soil science problems, with the exception of a brief summary of the present work, dealing only with the simpler van Genuchten model [16].

In this work, we present the details of the differential evolution method and we apply it to the calculation of the WRCs of soil samples with different texture, using the analytic models [1–3]. Differential evolution has been implemented in a Fortran command line application, *waterDE*, that can be run on any modern operating system.

The results obtained with waterDE have been assessed with RETC [17], the reference software package for the determination of WRCs from soil data. We show that, as with any NLS-based optimization method, the results of RETC depend on the initial choice of the model parameters, while waterDE can find the best set

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of characteristic parameters for the given experimental data independently of the random starting population of candidate solutions.

Due to their nature, NLS optimization methods can estimate the error of the calculated parameters, while heuristic optimization methods, such as differential evolution, do not intrinsically perform such error estimation. We have evaluated the error of the characteristic parameters calculated by waterDE through a stochastic approach based on the random perturbation of the experimental data.

2. Water retention models

Several analytic models have been proposed over the years to describe the WRC as accurately as possible in the widest range of suction. A comprehensive list of the available models can be found in [18].

Here we focus our attention on the three most widely used analytic models, that is those of van Genuchten [2], Brooks-Corey [1] and Rossi-Nimmo [3], in order of complexity of the representative equations. An extension of this work to other analytic models is straightforward.

2.1. van Genuchten model

The expression of the van Genuchten (VG) model is given by

$$\theta(\psi) = \theta_r + (\theta_s - \theta_r)\left[\frac{1}{1 + (\alpha|\psi|)^n}\right]^m \tag{1}$$

where θ_r is the residual water content, θ_s is the saturated water content, α is an empirical parameter related to the inverse of the air-entry suction ψ_e ($\alpha > 0$), n is a dimensionless parameter related to the distribution of pore sizes ($n > 1$) and m is a dimensionless parameter related to the symmetry of the model.

A simplified expression of the VG model is frequently used in water retention studies, where the m parameter is constrained to n through the relation $m = 1 - 1/n$. This is the form of VG model that will be used throughout this paper.

2.2. Brooks-Corey model

The Brooks-Corey (BC) model is expressed by

$$\theta(\psi) = \begin{cases} \theta_r + (\theta_s - \theta_r) & \text{for } \psi \leqslant \psi_e \\ \theta_r + (\theta_s - \theta_r)\left(\frac{\psi_e}{|\psi|}\right)^\lambda & \text{for } \psi > \psi_e \end{cases} \tag{2}$$

where ψ_e is the air-entry suction and λ is a dimensionless parameter related to the distribution of pore sizes ($\lambda > 0$).

2.3. Rossi-Nimmo model

The Rossi-Nimmo (RN) model is represented by the set of equations,

$$\theta(\psi) = \begin{cases} \theta_r + (\theta_s - \theta_r)\left[1 - \beta'\left(\frac{\psi}{\psi_e}\right)^2\right] & \text{for } 0 \leqslant \psi < \psi_i \\ \theta_r + (\theta_s - \theta_r)\left(\frac{\psi_e}{\psi}\right)^\lambda & \text{for } \psi_i \leqslant \psi < \psi_j \\ \theta_r + (\theta_s - \theta_r)\gamma' \ln\left(\frac{\psi_0}{\psi}\right) & \text{for } \psi_j \leqslant \psi \leqslant \psi_0 \end{cases} \tag{3}$$

where, in addition to the already defined parameters, ψ_0 is the maximum measured water suction, β' and γ' are shape parameters

$$\beta' = \frac{\lambda}{2}\left(\frac{2}{2+\lambda}\right)^{\frac{2+\lambda}{\lambda}} \tag{4}$$

$$\gamma' = \lambda \exp(1)\left(\frac{\psi_e}{\psi_0}\right)^\lambda \tag{5}$$

and ψ_i and ψ_j are the values of the suction at the two junction points of the RN function,

$$\psi_i = \psi_e\left(\frac{2}{2+\lambda}\right)^{-\frac{1}{\lambda}} \tag{6}$$

$$\psi_j = \psi_0 \exp(-1/\lambda) \tag{7}$$

3. Model optimization

The analytic models (1)–(3) depend on a vector of adjustable parameters $\mathbf{p}$, namely $\mathbf{p} = \{\theta_r, \theta_s, \alpha, n\}$ for the VG model and $\mathbf{p} = \{\theta_r, \theta_s, \psi_e, \lambda\}$ for either the BC or RN models, from which all the other parameters of Eqs. (4)–(7) can be calculated.

The best fit of a model to a measured WRC composed of N experimental points (observations) $\{\psi_i^o, \theta_i^o\}$, is calculated using an optimization method that minimizes the sum of the residuals,

$$\Delta(\mathbf{p}) \sim \sum_{i=1}^{N} \left|\theta_i^c - \theta_i^o\right|^2 \tag{8}$$

that is the squared deviation of the measured water content θ_i^o to the calculated water content $\theta_i^c = \theta(\psi_i^c, \mathbf{p})$, while satisfying at the same time the constraints imposed by the model, such as the bounding values of the model parameters. The parameter vector $\mathbf{p}$ that corresponds to the absolute minimum of $\Delta(\mathbf{p})$ gives the best agreement between the calculated WRC and the experimental data.

The optimization problem of Eq. (8) is usually solved using a NLS minimization method that, starting from an initial estimate of the model parameters, iteratively adjusts them until convergence is reached.

However, if the starting values of the model parameters are not reasonably close to the optimal (but still unknown) values, the optimization procedure might not converge or, whenever multiple local minima exist, it might get stuck in one of the local minima, instead of finding the desired global minimum of $\Delta(\mathbf{p})$.

NLS methods are also very sensitive to outliers. The presence of even a few outliers in the measured data gives a disproportionally large weight to the corresponding residuals of Eq. (8), seriously affecting the overall results of the optimization [19].

To improve the accuracy of the calculations and to reduce the effect of the outliers, NLS minimization methods need about 10 data points for each model parameter [20,21]. Usually this is not a strong limitation but, in this particular case, it means that for optimal results an experimental WRC should be composed of at least 40–50 observations, more or less evenly distributed from saturation to oven dryness, a range of suction covering several orders of magnitude.

Due to the complexity of the experimental procedure and to the necessity to wait to reach steady-state conditions before each measurement, the accurate hydraulic characterization of a porous medium is a long and error-prone process, that can take a few days or even weeks, depending on the medium under investigation and on the measurement method. Therefore, the number of experimental data points available in practice is usually much lower than the optimal number required by NLS methods.

With such small number of observations, several NLS (and also heuristic) optimization methods often struggle to find the optimal set of characteristic parameters for a given model, in particular when trying to characterize soils that cannot be easily classified in a standard textural class, such as for example poorly-graded soils or naturally occurring soils measured in the field, or also