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# A HYBRID SIMULATED ANNEALING AND GRADIENT-BASED ALGORITHM FOR THE ESTIMATION OF UNSATURATED SOIL PARAMETERS

# Luis Guarracino and Danilo Velis

CONICET, Facultad de Cs. Astronómicas y Geofísicas, Universidad Nacional de La Plata, Paseo del Bosque s/n, 1900 La Plata, Argentina, luisg@fcaglp.unlp.edu.ar, velis@fcaglp.unlp.edu.ar, http://www.fcaglp.unlp.edu.ar

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Abstract. Simulation of water flow in the unsaturated zone requires knowledge of hydraulic conductivity and water content functions. In most applied studies these functions are described by the well-known van Genuchten constitutive model, which has five independent parameters. Model parameters are usually determined from laboratory experiments, although often these estimates are non-representative of field conditions. In recent years, the use of inverse methods in conjunction with field experiments has become a promising alternative for the accurate estimation of unsaturated soil parameters. Essentially, this procedure involves the minimization of a cost or objective function that measures the discrepancy between observed and simulated data. In the present work we estimate the van Genuchten model parameters from hypothetical drainage experiments using a hybrid optimization strategy based on simulated annealing and a quasi-Newton method. Drainage experiments are modeled by solving Richards equation with appropriate initial and boundary conditions. To obtain approximate solutions of Richards equation we use a Galerkin finite element method. The algorithm behavior and the consequences on the estimated van Genuchten model parameters using different objective functions are explored. Objective functions are constructed from two sets of data which are usually obtained on field experiments: pressure head p versus time measured at different depths and water content  $\theta$  versus depth measured at different times. The proposed estimation procedure is tested using synthetically generated data. Numerical examples show that the inverse modeling of drainage experiments using a hybrid simulated annealing and gradient-based algorithm provides an excellent methodology for an efficient and accurate estimation of unsaturated soil parameters.

## **1 INTRODUCTION**

Modelling groundwater flow in the unsaturated zone using the continuum approach requires an accurate knowledge of the hydraulic conductivity K(h) and water content  $\theta(h)$  functions. These characteristic functions are usually described by empirical mathematical models with different number of fi tting parameters, such as Brooks-Corey (Brooks and Corey, 1964) or van Genuchten (van Genutchen, 1980) models. Traditionally, model parameters are determined from soil samples in the laboratory. Despite the sophistication and precision of laboratory procedures, estimated parameter are non-representative of fi eld conditions since the soil samples are small and in most cases the soil structure is disturbed (Kool et al., 1987). A promising alternative to laboratory methods is to determine unsaturated parameters by combining fi eld measurements with inverse methods of parameter optimization (Dane and Hurska, 1983; Zou et al., 2001; Simunek and van Genutchen, 1996; Olyphant, 2003).

Numerous optimization methods have been used for estimating unsaturated parameters such quasi-Newton (Zijlstra and Dane, 1996), Levenberg-Marquardt (Olyphant, 2003; Nutzmann et al., 1998), Simplex (Zou et al., 2001), Ant Colony (Abbaspour et al., 2001), and Adjoint Method (Santos et al., 2006). These methods minimize objective functions that measure the deviations between numerically predicted and observed data from laboratory or fi eld experiments. Inverse procedures generally work correctly, although they strongly depend on the objective function. In this context, the uniqueness of the solution may be in question (Zou et al., 2001; Carrera and Neuman, 1986).

The use of inverse methods allows more flexibility in the design of fi eld tests. One of the commonly used experiment to measure in situ water content  $\theta$  and pressure head p data is the unsteady drainage experiment (Green et al., 1986). This experiment is based on the saturation of the soil profi le and the subsequent measurement of the unsaturated variables during the drainage process. Soil profi le is fully or near fully saturated by adding water from the soil surface. Then the soil surface is covered with a plastic sheet to avoid evaporation and pressure head and water content values are measured with prescribed spatial and temporal sampling intervals. Soil water content is usually measured with a neutron probe while pressure head is measured using tensiometers (Zhang et al., 2003).

The objective of this paper is to present a hybrid optimization algorithm based on simulated annealing (SA) and a quasi-Newton method to determine unsaturated parameters from drainage experiments. The SA method is a stochastic computational algorithm for finding near optimal solutions to hard optimization problems. The quasi-Newton method is a gradient-based algorithm with quadratic convergence. Water flow in the soil profile during the drainage experiment is assumed to be described by the highly non-linear Richards equation (Richards, 1931) in conjunction with the well-known van Genuchten constitutive model. The objective function is constructed from measurement of pressure head p versus time at different depths and water content  $\theta$  versus depth at different times during the drainage experiment. The proposed optimization algorithm is used to estimate parameters of van Genuchten model. The performance of the algorithm and the uniqueness of the solutions is analyzed using synthetically generated data from hypothetical drainage experiments conducted in homogeneous and layered soil profiles.

The organization of the paper is as follows: in Section 2 we present Richards equation and initial and boundary conditions for describing drainage experiments, in Section 3 the estimation problem and the hybrid SA and gradient-based algorithm are presented. Finally, in Section 4 we show numerical examples and we analyze the performance of the proposed algorithm.

#### **2** THE DIRECT PROBLEM

We consider the problem of estimating unsaturated parameters from drainage experiments in a one-dimensional domain  $\Omega$  with boundary  $\partial \Omega$ . In the unsaturated zone water flow can be described by Richards equation (Richards, 1931) stated in the form

$$\frac{\partial}{\partial t}\theta(p) - \frac{\partial}{\partial z}\left[K(p)\frac{\partial}{\partial z}(p+z)\right] = 0, \quad z \in \Omega, \quad t \in I = (0,T), \tag{1}$$

with boundary conditions

$$-K(p)\frac{\partial}{\partial z}(p+z) = 0, \quad z \in \Gamma^*, \quad t \in I,$$

$$p = p^{bot}, \quad z \in \Gamma, \quad t \in I,$$
(2)

and initial condition

$$p(t=0) = p_0(z), \ z \in \Omega.$$
 (3)

In the equations above the *z*-axis is considered to be positive upward,  $\Gamma^*$  is the part of  $\partial\Omega$  associated with the top surface of the soil and  $\Gamma = \partial\Omega \setminus \Gamma^*$ . To solve the differential problem (1)–(3), we use the functions  $\theta(p)$  and K(p) given by the van Genuchten model (van Genutchen, 1980):

$$\theta(p) = \begin{cases} \frac{\theta_s - \theta_r}{[1 + (\alpha |p|)^n]^m} + \theta_r, & \text{for} \quad p < 0\\ \theta_s & \text{for} \quad p \ge 0, \end{cases}$$
(4)

$$K(p) = \begin{cases} K_s \frac{\{1 - (\alpha|p|)^{n-1}[1 + (\alpha|p|)^n]^{-m}\}^2}{[1 + (\alpha|p|)^n]^{m/2}} & \text{for} \quad p < 0\\ K_s & \text{for} \quad p \ge 0, \end{cases}$$
(5)

where  $\theta_r$  and  $\theta_s$  are the residual and saturated water contents, respectively;  $K_s$  is the saturated hydraulic conductivity; n and  $\alpha$  are shape parameters; and m is given by the relation m = 1 - 1/n.

Numerical solutions of the direct problem (1)-(3) are obtained using a Galerkin fi nite element procedure for space discretization combined with a backward Euler scheme in time. Non-linear terms of Richards equation are linearized using the modifi ed Picard iteration method proposed by Celia et al.(Celia and Bouloutas, 1990). The algorithm obtained with this approximation is computationally efficient and produces perfectly mass conservative numerical solutions.

#### **3** THE ESTIMATION PROBLEM

In this study we consider an objective function for parameter optimization based on the knowledge of the pressure head values versus time at some depths and water content values in the soil profile measured at different times. Let m be the set of unknown model parameters, which include  $K_s$ ,  $\alpha$ , n and  $\theta_s$  (for the purpose of this work, we assume that  $\theta_r$  is known)<sup>1</sup>. Also, let us define the objective function as:

$$\mathcal{J}(\mathbf{m}) = w\mathcal{J}_p(\mathbf{m}) + (1 - w)\mathcal{J}_\theta(\mathbf{m}),\tag{6}$$

<sup>&</sup>lt;sup>1</sup>Actually, note that **m** is a vector of 4N unknowns, where N is the number of layers used to parameterize the soil.

where  $\mathcal{J}_p(\mathbf{m})$  and  $\mathcal{J}_{\theta}(\mathbf{m})$  are terms based on pressure head and water content data, respectively, and  $w, 0 \le w \le 1$ , is a weighting factor.  $\mathcal{J}_p(\mathbf{m})$  and  $\mathcal{J}_{\theta}(\mathbf{m})$  are defined as follows:

$$\mathcal{J}_{p}(\mathbf{m}) = \left\{ \frac{1}{N_{dp}M_{t}} \sum_{j=1}^{M_{t}} \sum_{i=1}^{N_{dp}} \left[ p^{obs}(z_{i}, t_{j}) - p^{cal}(z_{i}, t_{j}) \right]^{2} \right\}^{1/2}$$
(7)

$$\mathcal{J}_{\theta}(\mathbf{m}) = 100 \left\{ \frac{1}{N_{tp}M_z} \sum_{j=1}^{M_z} \sum_{i=1}^{N_{ct}} \left[ \theta^{obs}(z_j, t_i) - \theta^{cal}(z_j, t_i) \right]^2 \right\}^{1/2},$$
(8)

where  $p^{obs}$  and  $p^{cal}$  are the observed and calculated pressure head values, respectively;  $N_{dp}$  is the number of depth points where pressure head is measured;  $M_t$  is the number of data points obtained at each depth  $z_i$ ;  $\theta^{obs}$  and  $\theta^{cal}$  are the observed and calculated water content values, respectively;  $N_{tp}$  is the number of time points where water content is measured, and  $M_z$  is the number of data points obtained at each time  $t_i$ .

So, given a set of observations (pressure head and/or water content), the estimation problem consists on finding the set of unknown parameters  $\mathbf{m} = (K_s, \alpha, n, \theta)$  that, when input into the direct problem described in the previous section, yield calculated pressure head and/or water content values that fit the data observations within a given tolerance. Clearly, this is a highly nonlinear inverse problem that should be solved iteratively. Further, it represents a *constrained* nonlinear inverse problem, since model parameters have physical meaning only for a given range. In complex situations (e.g. soils represented by more that one layer, each layer made up of distinct materials), if a good initial guess for  $\mathbf{m}$  is not available, standard optimization algorithms (in general based on gradient directions) are prone to converge to local minima or even diverge, because they make downhill moves only.

On the contrary, in SA optimization uphill moves are not forbidden, thus local minima can be avoided and the global minimum can be effectively reached. The price to be paid is computational cost, since usually SA requires a large number of iterations for convergence. In practice, we minimize  $\mathcal{J}(\mathbf{m})$  using a hybrid strategy that combines simulated annealing (SA) optimization with a gradient-based optimization procedure. This hybrid strategy will be described in next subsections.

Another issue worth mentioning is the reason of using an objective function that combines two different terms, one based on pressure head observations, and the other based on water content observations. As it will be shown later, if data observations are based on pressure head only, these measurements are generally not enough to determine the soil model parameters uniquely. That is, there are several model parameters sets that fit the data equally well. This nonuniqueness problem (which is inherent to many nonlinear inverse problems) can be eliminated by using an objective function which is based on water content, too. Further, measurements based on water content only may be enough to uniquely determine the model parameters in simple soil models (thus pressure head observations are not needed at all). However, in complex soil models we found it useful to make use of both types of observations. For this purpose we introduced the weighting factor w in equation (6).

#### 3.1 Simulated annealing

The simulated annealing (SA) method is a stochastic computational algorithm for finding near optimal solution to hard optimization problems. The basic concept of the SA strategy is derived from the process of annealing in thermodynamics (Metropolis et al., 1953; Kirkpatrick et al.,

1983). The slow cooling of a molten material allows the reorientation of particles to form large crystals and this state is visualized as being equivalent to the global minimum of the energy of the system. On the other hand, the rapid cooling results in formation of glass and this state is considered as being one of the many possible local minima.

In SA optimization, the unknown parameters play the role of the particles in the molten material, and the objective function represents the energy of the system. Here, parameter values (i.e. new model states) are drawn from a distribution that depends on a control temperature, which is gradually decreased. At high temperatures, the model space is sampled more or less uniformly. But at low temperatures, models with lowest energy are preferably sampled. The model is updated using the Metropolis criterion (Metropolis et al., 1953) to decide whether to accept or reject the proposed model according to the change in the objective function value. Finally, convergence is achieved at low temperatures when no further improvement in the objective function is observed. The key of SA optimization is that when the objective function decreases, the proposed model is accepted unconditionally. On the other hand, when the objective function increases, it is accepted with a probability greater than zero (the higher the temperature, the higher the probability). This strategy allows SA to easily escape local minima.

SA comes in various flavors. Here we use one of the most powerful SA approaches, which is called very fast simulated annealing (VFSA) (Ingber, 1993). The advantage of VFSA over traditional SA techniques relies on the choice of the generating distribution and the cooling schedule. For selecting new parameter values, VFSA uses a long-tailed Cauchy-like distribution that permits the exploration of the model space more effectively than using Gaussian or uniform distributions (Ingber, 1993), as in various SA algorithms. Also, a faster cooling rate is allowed to accelerate convergence without limiting its ability to avoid local minima. At iteration k, the temperature associated with each parameter is given by

$$T_k = T_0 e^{-ck^{1/M}}, (9)$$

where  $T_0$  is the initial temperature, M is the number of unknowns, and c is a user-defined constant that can be used to tune the algorithm. The temperature associated to the objective function (the one used by the Metropolis rejection/acceptance criterion) is defined similarly to the parameter temperature. A further feature of VFSA is that parameter temperatures can be adapted dynamically ("re-annealing") according to the sensitivity of the objective function to each dimension in the model space, thus allowing for a different annealing schedule for each parameter. The reader is referred to the works by Ingber (1989, 1993) for a detailed description of VFSA.

## 3.2 Hybrid strategy

Despite the fact that VFSA converges significantly faster than conventional SA methods, when  $\mathcal{J}(\mathbf{m})$  is close to the global minimum, reducing it to zero (within a given tolerance) may take several iterations. At these low temperature stages, we found it convenient to switch to a gradient-based optimization algorithm to find the optimum model parameters more accurately and efficiently. Here, the best SA solution obtained so far is used as the initial guess for the linearizing stage. The switch is done after the maximum number of SA iterations has been reached. This hybrid strategy allows the proposed estimation procedure to accurately obtain the global minimum in an efficient manner. Since the gradient-based optimization algorithm is applied only after SA has converged close enough to the global minimum, problems regarding instability and divergence associated with these methods are of no concern. Locally,  $\mathcal{J}(\mathbf{m})$  is a

well-behaved function, and the convergence to the global minimum is guaranteed.

Any linearizing (or gradient-based) method can be used to minimize equation (6). At the beginning of the  $j^{\text{th}}$  iteration, the current model parameter estimates are  $\mathbf{m}^{j}$ . Essentially, the  $j^{\text{th}}$  iteration then consists of the computation of a search vector  $\Delta \mathbf{m}^{j}$  from which to obtain the new estimate  $\mathbf{m}^{j+1}$  according to  $\mathbf{m}^{j+1} = \mathbf{m}^j + \beta^j \Delta \mathbf{m}^j$ , where the step-size  $\beta^j$  is obtained by linear search or other strategy. The selection of the search vector is largely what distinguishes one method from another. In the method of steepest descent, for example, the greatest reduction in the objective function value is obtained in the direction of the negative gradient. But steepest descent method is known to have poor convergence ratios when the function to be minimized has long and narrow valleys, even when these valleys are perfectly quadratic. Contrarily, variable-metric methods (also known as quasi-Newton methods), are devised to obtain the exact minimum of a quadratic form in M dimensions after successive line minimizations. Like in conjugate gradient methods, it is assumed that the function to be minimized can be locally approximated by a quadratic form. This requires the knowledge of the gradient vector (first derivatives) and the Hessian matrix (second derivatives). The key of variable-metric methods relies on the fact that they manage to build iteratively a good approximation of the Hessian matrix after M line minimizations, which is often better than using the true Hessian(Press et al., 1992). Thus, the Hessian matrix is not required at all, and only first derivatives need to be calculated.

In practice, we estimate the fi rst derivatives required by the quasi-Newton method using fi nite differences. Consequently, only forward computations are performed throughout the iterative estimation process. In our experiments, usually 10-20 iterations are enough to reduce  $\mathcal{J}(\mathbf{m})$  to very small values and to guarantee that data observations are honored very accurately.

# **4 NUMERICAL EXPERIMENTS**

In this section the performance of the optimization algorithm presented above is analyzed using different combinations of measured data for both homogeneous and layered soil profiles.

#### 4.1 Parameter estimates for a homogeneous soil profile

In order to assess the influence of the different parts of objective function (6) on parameter estimates, we consider a hypothetical drainage experiment in a homogeneous soil profile. Synthetic data are generated by solving the direct problem with the van Genuchten parameters obtained by Carsel and Parrish (Carsel and Parrish, 1988) for a loamy sand texture (parameters are listed in Table 1).

Pressure head values are assumed to be measured at depths of 50, 100 and 150 cm ( $N_{dp} = 3$ ) at time intervals of 3 hours during a 24 hours drainage test ( $M_t = 8$ ). Water content values are obtained at t = 0.1, 0.3, 0.6 days ( $N_{tp} = 3$ ) with a sampling interval of 25 cm ( $M_z = 8$ ).

To evaluate the influence of the term  $\mathcal{J}_{\theta}$  in parameter estimates we set w = 0 in the objective function (6). This choice implies that only water content data are considered in the estimation of unsaturated parameters. After 50 iterations of VFSA and 20 iterations of quasi-Newton method the assumed values for van Genuchten parameters are exactly recovered. The excellent agreement between predicted and theoretical values of pressure head and water content is shown in Figure 1.

The influence of term  $\mathcal{J}_p$  in parameter estimates is analyzed by setting w = 1 in objective function (6). For this option, the estimation procedure is based only on pressure head values. The true values of  $K_s$  and  $\alpha$  parameters are not recovered (see Table 1) even though the agree-



Figure 1: a) Theoretical (crosses) and predicted (continuous lines) values of p using  $J_{\theta}$ ; b) Theoretical (crosses) and predicted (continuous lines) values of  $\theta$  using  $J_{\theta}$ .

ment between predicted and theoretical values of pressure head is very good (Figure 2a). As shown in Figure 2b, water content values (which are not included in the objective function) do not fit the theoretical values.



Figure 2: a) Theoretical (crosses) and predicted (continuous lines) values of p using  $J_p$ ; b) Theoretical (crosses) and predicted (continuous lines) values of  $\theta$  using  $J_p$ .

	$K_s$ (cm/s)	$\alpha$ (1/cm)	n	$\theta_s$	$ heta_r$
true values	0.001228	0.075	1.89	0.41	0.065
estimated values	0.001750	0.086	1.89	0.41	0.065

Table 1: True and estimated unsaturated parameters using  $J_p$ .

To test the uniqueness of the inverse solution of the parameter optimization procedure, we analyze the objective function in the parameter space. Figure 3 shows plots of  $\mathcal{J}_p$  and  $\mathcal{J}_{\theta}$  in the  $K_s$ - $\alpha$  plane. True values of  $(K_s, \alpha)$  and estimated values obtained using  $\mathcal{J}_p$  are indicated with crosses in both plots. The objective function  $\mathcal{J}_p$  shows a long valley which indicates the non-uniqueness of the inverse solution since there are many combinations of parameters that can accurately predict pressure head values. On the other hand, the objective function  $\mathcal{J}_{\theta}$  shows a well-defi ned global minima which allows the recovery of true parameters, as it was shown in the previous example.



Figure 3: a) Logarithm of  $J_p$  in the  $K_s$ - $\alpha$  plane; b)  $J_{\theta}$  in the  $K_s$ - $\alpha$  plane

### 4.2 Parameter estimates for a layered soil profile

In this numerical example we test the ability of the proposed algorithm to estimate the unsaturated parameters in a layered soil profi le. The soil profi le consists of three layers whose depth, class texture and van Genuchten parameter values are listed in Table 2. Pressure head values are assumed to be measured at depths of 45, 125 and 200 cm ( $N_{dp} = 3$ ) at time intervals of 3 hours during a 24 hours drainage test ( $M_t = 8$ ). Water content values are obtained at t = 0.1, 0.4, 0.8days ( $N_{tp} = 3$ ) with a sampling interval of 30 cm ( $M_z = 9$ ).



Figure 4: a) Theoretical (crosses) and predicted (solid lines) values of p; b) Theoretical (crosses) and predicted (solid lines) values of  $\theta$ 

Motivated by the results of the previous example we give more weight to the term  $\mathcal{J}_{\theta}$  by selecting a weighting factor w = 0.2. The optimization procedure achieved the prescribed tolerance in 500 iterations of VFSA and 100 iterations of quasi-Newton method. The excellent agreements between predicted and theoretical values of both pressure head and water content are shown in Figure 4. The estimated values of unsaturated parameters are very close to the real values (compare values of Tables 2 and 3).



Figure 5: a) Convergence after 500 iterations of VFSA (continuous line) and 100 iterations of quasi-Newton (dashed line); b)  $K_s$  versus iteration; c)  $\alpha$  versus iteration; d) n versus iteration; e)  $\theta_s$  versus iteration. Dashed black lines are real values.

Figure 5a illustrates the objective function versus iteration number. Note that the convergence of the algorithm is accelerated from iteration number 500 when the optimization is switched from SA to the quasi-Newton method. Finally, the convergences of estimated parameters are shown in Figures 5b-e. In all cases, estimated parameters are very close to the true values after 500 VFSA iterations (continuous lines), and true values are achieved after 100 quasi-Newton iterations (dashed lines). It is worth mentioning that convergence was not possible using the quasi-Newton method alone unless a very good initial guess for all the unknonw parameters was available. In most cases, the algorithm converged to local minima corresponding to wrong soil parameters.

# 5 CONCLUSION

Determining unsaturated parameters from field experiments using optimization methods is often difficult because the inverse problem is highly nonlinear and solutions are not unique. In this paper, we propose a hybrid optimization strategy based on simulated annealing and a

	Texture	depth (cm)	$K_s$ (cm/s)	$\alpha$ (1/cm)	n	$\theta_s$	$ heta_r$
Layer 1	silt loam	0 < z < 90	0.000125	0.020	1.41	0.45	0.067
Layer 2	sandy clay loam	90 < z < 160	0.0003638	0.059	1.48	0.39	0.10
Layer 3	loam	160 < z < 240	0.0002888	0.036	1.56	0.43	0.078

Table 2: Textures, depths and van Genuchten parameters obtained by (Carsel and Parrish, 1988)

	$K_s$ (cm/s)	$\alpha$ (1/cm)	n	$\theta_s$
Layer 1	0.000127	0.0200	1.4104	0.4500
Layer 2	0.000366	0.0589	1.4837	0.3900
Layer 3	0.000288	0.0369	1.5605	0.4299

Table 3: Estimated unsaturated parameters.

quasi-Newton method for determining van Genuchten parameters from drainage experiments. The objective function is constructed from both pressure head and water content data. Numerical examples for homogeneous soil profiles show that the addition of water content data in the objective function greatly improved the definition of a global minima. The performance of the proposed algorithm was successfully tested also in layered soil profiles. From the numerical results we can conclude that the proposed metodology is a promising tool for in situ estimation of unsaturated parameters. However, the utility of this procedure to estimate unsaturated parameters from real data has yet to be proven.

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