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A FULL-NEWTON ALGORITHM FOR PARAMETER ESTIMATION IN UNSATURATED SOILS

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Abstract. An iterative algorithm based on a full-Newton method for the estimation of the saturated hydraulic conductivity k in the unsaturated zone from drainage experiments is presented. The groundwater flow is assumed to be described by Richards equation and the well-known van Genuchten constitutive model. The cost functional used for the parameter optimization is defined as the L^2-error between the calculated pressure head values and the observed data at discrete points in the soil profile during the drainage process. The derivative of pressure head with respect to the parameter k is obtained as the solution of a differential equation with appropriate boundary and initial conditions. A Galerkin finite element procedure is used to obtain approximated solutions of the two differential problems involved in each iteration: the direct problem and the derivative of the functional. The algorithm was implemented in one-dimensional domains and used to estimate k in layered soil using synthetically generated data. Numerical examples show that the proposed algorithm yields very good estimations of the saturated hydraulic conductivity and becomes a promising method for *in situ* estimation of this parameter.

1 INTRODUCTION

Numerical simulation of unsaturated flow requires an accurate knowledge of the hydraulic conductivity and water content functions. These characteristic functions are usually described by empirical mathematical models with different number of fitting parameters, such as Brooks-Corey (Brooks and Corey, 1964) or van Genuchten (van Genutchen, 1980) models. Model parameters are usually determined from laboratory experiments, but these parameter values are often non-representative of field conditions. In recent years, inverse methods of parameter optimization applied to field experiments have became popular and appear promising. (Dane and Hurska, 1983; Zou et al., 2001; Simunek and van Genutchen, 1996; Olyphant, 2003). Various optimization methods such Simplex (Zou et al., 2001), quasi-Newton (Zijlstra and Dane, 1996), Adjoint Method (Santos et al., 2006), Ant Colony (Abbaspour et al., 2001) and Levenberg-Marquardt (Olyphant, 2003; Nutzmann et al., 1998) have been used for parameter estimation of unsaturated parameters. In particular, the estimation of the saturated hydraulic conductivity k is rather critical because the groundwater flow is highly sensitive to this parameter (Dane and Molz, 1991). It is important to remark that hydraulic conductivity values are relatively easy to obtain from laboratory methods, but these values are often non-representative of *in-situ* conditions (Kool et al., 1987).

The objective of this paper is to present an optimization algorithm based on a full-Newton method to determine the saturated hydraulic conductivity field from drainage experiments. Groundwater flow is assumed to be described by Richards equation (Richards, 1931) in conjunction with the well-known van Genuchten model. The optimization problem minimizes the L^2-error between the pressure head values p calculated at measurement points and the measured values of the pressure head. The proposed algorithm requires the calculation of the derivative of the pressure head with respect to the parameter k at each iteration level. This derivative is defined at the continuous level as the solution of a partial differential equation with appropriate initial and boundary conditions and then discretized using a finite element procedure. This approach, known as *differentiate-then-discretize*, provides an expression for the derivative which is independent of the particular discretization algorithm used to solve the differential problem. This method has been used for example, in (Tarantola, 1984, 1987; Fenandez-Berdaguer et al., 1993, 1995) to solve parameter estimation problems in geophysics and other applications. For an account of several aspects of estimation such as regularization, identifiability, etc, we refer to (Banks and Kunish, 1989). In particular, the proposed procedure allows for a more accurate calculation of derivatives of the cost functional than the standard *discretize-then-differentiate* approach consisting in discretizing the differential equations first and then applying optimization techniques to a discrete version as described for example in (Lines and Treitel, 1984).

The organization of the paper is as follows: in Section 2 the direct model and the estimation problem are presented. In Section 3 the full-Newton algorithm and its implementation is stated. Finally, a numerical example for a drainage test in a stratified sandy loam soil is presented in Section 4.

2 THE DIRECT MODEL AND THE ESTIMATION PROBLEM

2.1 The direct model

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

$$\frac{\partial}{\partial t}\theta\left(p(k)\right) - \nabla \cdot [kg(p(k))\nabla(p(k)+x)] = 0, \quad x \in \Omega, \quad t \in I = (0,T), \tag{1}$$

with boundary conditions

$$\begin{aligned} &-kg(p(k))\nabla(p(k)+x)\cdot n = q^*, \quad x \in \Gamma^*, \quad t \in I, \\ &p(k) = p^{bot}, \quad x \in \Gamma, \quad t \in I, \end{aligned} \tag{2}$$

and initial condition

$$p(k)(t=0) = p_0(x),\ x \in \Omega. \tag{3}$$

In the equations above the x-axis is considered to be positive upward, Γ^* 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), the functions $\theta(p)$ and $g(p)$ need to be specified. One of the commonly used pairs $(\theta(p), g(p))$ is given by the van Genuchten model (van Genutchen, 1980):

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

$$g(p) = \begin{cases} \dfrac{\{1-(\alpha|p|)^{n-1}[1+(\alpha|p|)^n]^{-m}\}^2}{[1+(\alpha|p|)^n]^{m/2}} & \text{for} \quad p < 0 \\ 1 & \text{for} \quad p \geq 0, \end{cases} \tag{5}$$

where θ_r and θ_s are the residual and saturated water contents, respectively; n and α are shape parameters; and m is given by the relation $m = 1 - 1/n$.

2.2 The estimation problem

For the estimation problem we assume that the saturated hydraulic conductivity $k(x)$ belongs to the set

$$\mathcal{P}^M = \left\{ k(x) : k(x) = \sum_{j=1}^{M} k_j \psi_j(x), \quad k_* \leq k_j \leq k^*, \quad x \in \Omega \right\}$$

where $\psi_j(x)$ denotes the characteristic function of the interval (x_{j-1}, x_j), and k_*, k^* are positive constants. We also assume that the pressure head values p are recorded at the points x_{ri}, $1 \leq i \leq N_r$, inside Ω for all $t \in I$.

Let us define the cost functional as

$$\mathcal{J}(k) = \frac{1}{2}\|p(k) - p^{obs}\|_{L^2(I,R^{N_r})} \tag{6}$$

where $p^{obs} = ((p(x_{ri}, t))_{1\leq i\leq N_r}$ is the observation vector. In this case, the estimation problem can be formulated as follows:

$$\text{minimize} \quad \mathcal{J}(k) \quad \text{over} \quad \mathcal{P}^M. \tag{7}$$

A common difficulty in solving problem (7) is that the cost functional $\mathcal{J}(k)$ is not generally convex. In order to overcome this situation, we add a regularization term and we define a new functional cost as follows:

$$\mathcal{J}^\beta(k) = \frac{1}{2}\|p(k) - p^{obs}\|_{L^2(I,R^{N_r})} + \frac{1}{2}\beta\|k - k_{ref}\|^2_{L^2(\Omega)} \tag{8}$$

where β is a regularization parameter and k_{ref} is a reference value for k. Note that minimizations of $\mathcal{J}(k)$ and $\mathcal{J}^{\beta}(k)$ are different problems. However, it can be proven that under certain hypothesis the minimum k of $\mathcal{J}^{\beta}(k)$ as $\beta \to 0$ approaches the minimum k of $\mathcal{J}(k)$ (Banks and Kunish, 1989). Then, our estimation problem will be:

$$\text{minimize} \quad \mathcal{J}^{\beta}(k) \quad \text{over} \quad \mathcal{P}^M \quad \text{as} \quad \beta \to 0. \tag{9}$$

3 THE ESTIMATION ALGORITHM

The Newton method requires the computation of derivative $D_k(p)$ of the solution $p(k,x,t)$ of (1)–(3) with respect to the parameter function $k(x)$. According with (2.2) $k(x)$ is a step function of the form $k(x) = \sum_{j=1}^{M} k_j \psi_j(x)$ and it can be identified with the vector $\mathbf{k} = (k_1, k_2, ..., k_M) \in R^M$.

The linear operator $D_k(p)$ is completely determined by the functions:

$$D_k(p)\psi_j(\cdot,\cdot) \equiv D_k^j(p,\cdot,\cdot), \; 1 \le j \le M \tag{10}$$

defined as solutions of the differential equation

$$\begin{aligned} &\frac{\partial}{\partial t}\left(\frac{\partial \theta}{\partial p} D_k^j(p)\right) - \nabla \cdot \left(kg(p)\nabla D_k^j(p)\right) - \nabla \cdot \left(k\frac{\partial g}{\partial p} D_k^j(p)\nabla(p+x)\right) \\ &= \nabla \cdot (g(p)\psi_j \nabla(p+x)), \quad x \in \Omega, \quad t \in I = (0,T), \end{aligned} \tag{11}$$

with boundary conditions

$$\begin{aligned} &-kg(p)\nabla D_k^j(p)\cdot n = -\frac{\partial g}{\partial p} D_k^j(p)\frac{q^*}{g(p)} - \frac{\psi_j q^*}{k}, \quad x \in \Gamma^*, \quad t \in I, \\ &D_k^j(p) = 0, \quad x \in \Gamma, \quad t \in I, \end{aligned} \tag{12}$$

and initial condition

$$D_k^j(p)(t=0) = 0, \; x \in \Omega. \tag{13}$$

Next we motivate the parameter estimation algorithm. Let k_0 be an initial estimation of the parameter. Set $k_{ref} = k_0$ in the regularization term (8) and $\delta k = k - k_0$. Assume that the cost functional $J^{\beta}(k)$ has a minimum at $k_0 + \delta k$; thus we want to compute δk. Since $k_0 + \delta k$ is a minimum for J^{β} then

$$\left.\frac{\partial J^{\beta}}{\partial k}\right|_{k_0+\delta k} = 0. \tag{14}$$

A first order approximation of (14) can be written in the form:

$$\left\{\int_0^T \left[\mathbf{D}_{k_0}(p)\right]^t(\tau)\mathbf{D}_{k_0}(p)(\tau)d\tau + \beta\Lambda\right\}\delta\mathbf{k} = \int_0^T \left[\mathbf{D}_{k_0}(p)\right]^t(\tau)\left(p^{obs}(\cdot,\tau) - p(k_0,\cdot,\tau)\right)d\tau \tag{15}$$

where $\mathbf{D}_k(p)(t) \in R^{1\times M}$ is the row-vector with components$(D_k(p)(t))_j = D_k^j(p, x_r, t), \; 1 \le j \le M$, $\Lambda = \text{diag}(|\Omega_1|, |\Omega_2|, ..., |\Omega_M|)$, and $\delta\mathbf{k} = (\delta k_1, \delta k_2, ..., \delta k_M)$.

Note that using (15) we can determine $\delta\mathbf{k}$, and this suggest the following iterative algorithm:

$$\mathbf{k}^{(i+1)} = \mathbf{k}^{(i)} + \delta\mathbf{k}^{(i+1)} \tag{16}$$

with

$$\delta \mathbf{k}^{(i+1)} = \left[\mathbf{M}^{\beta(i)}(\mathbf{k}^{(i)})\right]^{-1} \mathbf{H}^{\beta(i)}(\mathbf{k}^{(i)}), \tag{17}$$

where $\mathbf{M}^{\beta}(\mathbf{k})$ and $\mathbf{H}^{\beta}(\mathbf{k})$ are defined as

$$\mathbf{M}^{\beta}(\mathbf{k}) = \int_0^T \left[\mathbf{D}_k(p)\right]^t(\tau)\mathbf{D}_k(p)(\tau)d\tau + \beta\Lambda \tag{18}$$

$$\mathbf{H}^{\beta}(\mathbf{k}) = \int_0^T \left[\mathbf{D}_k(p)\right]^t(\tau)\left(p^{obs}(\cdot,\tau) - p(k,\cdot,\tau)\right)d\tau. \tag{19}$$

The main difference between the technique presented here and the usual discrete methods is based on the calculation of the derivative of the pressure head with respect to the parameter k. In this paper we compute $D_k(p)$ by solving system (11)–(13) while discrete methods use incremental quotients.

The minimization procedure can be stated as follows:

- 1) Set $i = 0$ and give an initial guess $k = k_0(x)$.
- 2) Compute $p(k)$ by solving (1)-(3).
- 3) Compute $D_k^j(p)$ by solving (11)–(13).
- 4) Determine $\delta\mathbf{k}$ by solving (17).
- 5) Update the saturated hydraulic conductivity $\mathbf{k}^{(i+1)} = \mathbf{k}^{(i)} + \delta\mathbf{k}^{(i+1)}$
- 6) Compute error, if convergence is achieved, stop.
- 7) New iteration: set $i = i + 1$ and go to 2).

The numerical solutions of the direct problem (1)-(3) and the derivatives (11)-(13) were obtained using Galerkin finite element procedures. Mathematical results concerning the convergence of the algorithm are presented in (Fenandez-Berdaguer et al., 1993).

4 NUMERICAL EXPERIMENT

The proposed algorithm was implemented to estimate the saturated hydraulic conductivity $k(x)$ in a vertical heterogeneous soil profile during a drainage experiment using synthetically generated data. The observed data p^{obs} are the pressure head values versus time at different depths obtained as the solution of the forward problem.

For the numerical test we consider a 200 cm sandy loam soil profile consisting of four layers with the following values of $k(x)$

$$k(x) = \begin{cases} 120 \text{ cm/day} & 0 \text{ cm} \leq x < 50 \text{ cm} \\ 60 \text{ cm/day} & 50 \text{ cm} \leq x < 100 \text{ cm} \\ 90 \text{ cm/day} & 100 \text{ cm} \leq x < 150 \text{ cm} \\ 150 \text{ cm/day} & 150 \text{ cm} \leq x \leq 200 \text{ cm}. \end{cases} \tag{20}$$

The other hydraulic parameters of van Genuchten model for a sandy loam soil are assumed to be constant over the whole profile with θ_s = 0.41, θ_r = 0.065, n = 1.89 and α = 0.075 cm^{-1} (Carsel and Parrish, 1988).

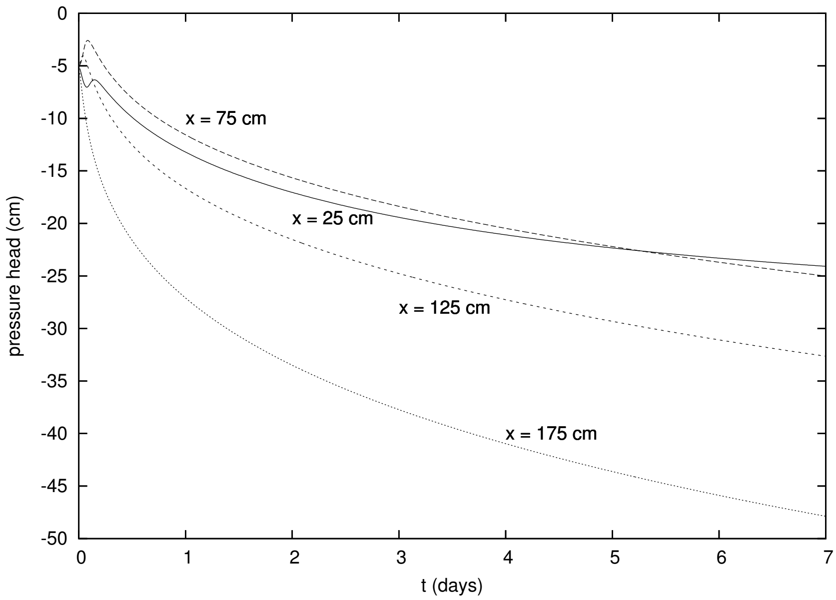

Figure 1: Simulated pressure head observations at $x = 25, 75, 125$ and 175 cm depths.

In a drainage experiment, the soil profile is previously saturated from the soil surface. Water is added until all tensiometers indicate fully saturated conditions. At this point, the soil surface is covered with a plastic sheet to avoid evaporation and water begins to drain under gravity. During the drainage process pressure head values are continuously measured using tensiometers until the end of the experiment (Chena and Payne, 2001).

The boundary and initial conditions for the drainage experiment explained above are:

$$-kg(p)\nabla(p+x)\cdot n = 0, x \in \Gamma^*, \quad t \in I \tag{21}$$

$$p = 0, \quad x \in \Gamma, \quad t \in I,$$

$$p(t=0) \approx 0\,(p<0), \quad x \in \Omega. \tag{22}$$

The time step used in the numerical solution of direct problem (1)-(3) and the derivatives (11)-(13) is $\Delta t = 864$ s with a uniform partition of Ω into elements of size $h = 3.33$ cm.

The pressure head values are assumed to be recorded at discrete times t_n at 4 points x_{ri} spaced 50 cm from each other. Figure 1 shows simulated pressure head observations at the recording points x = 25 cm, 75 cm, 125 cm and 175 cm.

The initial guess for $k(x)$ in the inverse procedure is taken to be constant an equal to 105 cm/day. The regularization parameter β is chosen to be proportional to the cost functional and inversely proportional to the variance of the estimated hydraulic conductivity. Using this β the algorithm achieves the prescribed tolerance in 27 iterations. Figure 2 shows the initial guess and the estimated profiles of $k(x)$. Figure 3 illustrates the behavior of the cost functional against number of iterations. The full-Newton algorithm gives a very good estimate of k, even though there is only one observation point in each layer.

5 CONCLUSIONS

A full-Newton algorithm to estimate the saturated hydraulic conductivity in one-dimensional layered unsaturated soils is presented. The derivatives of pressure head with respect to parameter k are computed by solving a differential equation. This allows to solve the estimation

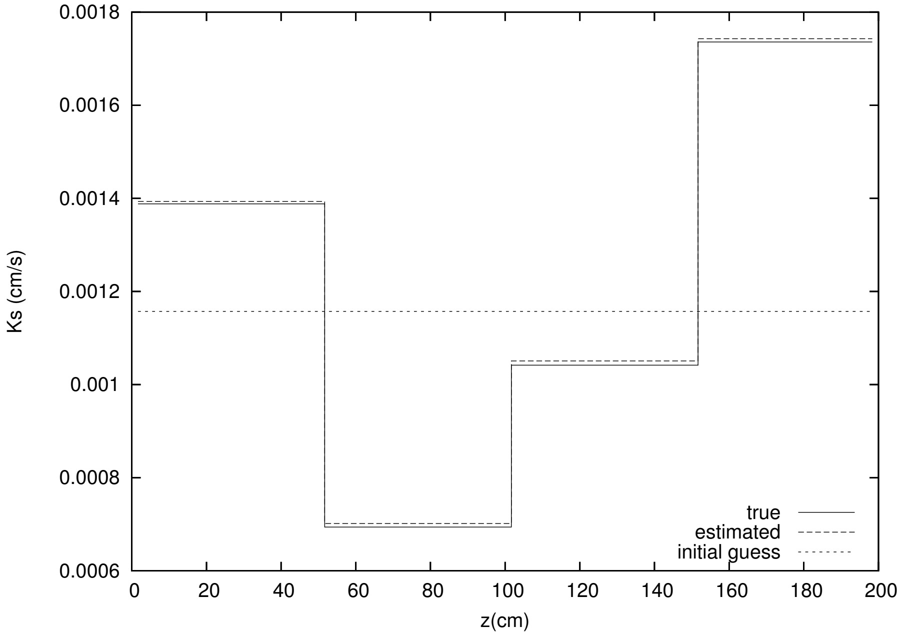

Figure 2: Initial, estimated (dashed) and true (continuous) hydraulic conductivity.

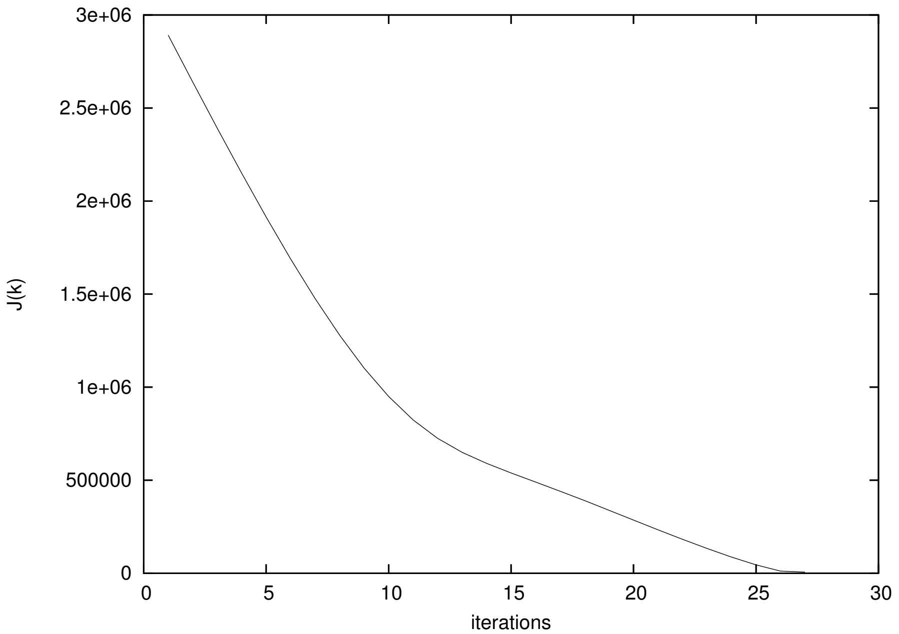

Figure 3: Cost functional.

problem independently of the discretization scheme used to solve the associated partial differential equations. In the present work standard Galerkin procedures were employed to solve differential problems involved in each iteration. From the numerical example shown in Section 4, we can conclude that the proposed algorithm yields a very good estimate of saturated hydraulic conductivity in a stratified medium and becomes a promising method for *in situ* estimation of this parameter. The full-Newton algorithm is currently being generalized to include the estimation of the other unsaturated parameter of van Genuchten constitutive model.

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