Mecánica Computacional Vol. XXIV
A. Larreteguy (Editor)
Buenos Aires, Argentina, Noviembre 2005

NUMERICAL EXPERIMENTS ON HYDRAULIC CONDUCTIVITY ESTIMATION USING THE ADJOINT METHOD

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Key Words: Inverse problem, Adjoint method, hydraulic conductivity.

Abstract. *An iterative algorithm based on the adjoint method for the estimation of the saturated hydraulic conductivity k in the unsaturated zone from infiltration 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 infiltration process. The exact gradient of the cost functional is obtained by solving an appropriate adjoint problem, which is derived from the equations of the Gâteaux derivatives of the pressure head with respect to the parameter k. The optimization procedure is solved employing a nonlinear conjugate gradient method. A Galerkin finite element procedure is used to obtain approximated solutions of the three differential problems involved in each iteration: the direct and the adjoint problems and the Gâteaux derivatives. The algorithm was implemented in one-dimensional domains and used to estimate k in heterogeneous soil profiles 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 modeling of soil moisture 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[1] or van Genuchten[2] models. Model parameters are often difficult or even impossible to measure directly because of instrumentation, scale or conceptual constraints. Thus, inverse modeling of laboratory or field data has become an attractive alternative to direct measurements.[3–6] In recent years, various optimization methods such quasi-Newton,[7] Simplex,[4] Levenberg-Marquardt[6,8] and Ant Colony[9] have been used for parameter estimation of characteristic curves. In particular, the estimation of the saturated hydraulic conductivity is rather critical because the groundwater flow is highly sensitive to this parameter.[10] Hydraulic conductivity values are relatively easy to obtain from laboratory methods but these values are often non-representative of *in-situ* conditions.[11]

The objective of this paper is to present a nonlinear optimization algorithm to determine the saturated hydraulic conductivity field first described in.[12] Groundwater flow is assumed to be described by Richards equation[13] in conjunction with the well-known van Genuchten model. The optimization problem minimizes the L^2-error between the pressure head values $p(x, k, t)$ calculated at the measurements points and the measured values of the pressure head at these discrete points. The gradient of the cost functional in our nonlinear optimization problem is defined at the continuous level using the adjoint of the Gâteaux derivative of the solution with respect to the parameter. Both the Gâteaux derivative and the adjoint are defined at the continuous level as solutions of partial differential equations with appropriate initial and boundary conditions and then discretized using finite element procedures. This approach, known as *differentiate-then-discretize*, provides an expression for the gradient which is independent of the particular discretization algorithm used to solve the differential problems. This method has been used for example, in[14–19] 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.[20] In particular, the proposed adjoint procedure allows for a more accurate calculation of the gradient 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.[21]

The organization of the paper is as follows: in Section 2 the direct model, the inverse problem and the sensitivity equations are presented. In Section 3 the algorithm and its implementation is stated. Finally, in Section 4 a numerical example is presented.

2 THE DIRECT MODEL, THE ESTIMATION PROBLEM AND THE SENSIVITY EQUATIONS

2.1 The direct model

We consider the problem of estimating the saturated permeability $k(x)$ in a multidimensional bounded variably saturated soil Q with boundary ∂Q. Let Γ^* be the part of ∂Q associated with the top surface of the soil, i.e., the part of ∂Q, where the rain and evapotranspiration data will be specified and we set $\Gamma = \partial Q \setminus \Gamma^*$.

It will be assumed that water flow within Q is governed by Richards equation[13] stated in the form

$$D_t\theta(p(k)) - div(kg(p(k))D_x(p(k) + x_3)) = 0, \quad x \in Q, \quad t \in I = (0, T), \tag{1}$$

with boundary condition

$$\begin{aligned} -kg(p(k))D_x(p(k) + x_3) \cdot n = q^*, \quad x \in \Gamma^*, \quad t \in I, \\ -kg(p(k))D_x(p(k) + x_3) \cdot n = 0, \quad x \in \Gamma, \quad t \in I, \end{aligned} \tag{2}$$

and initial conditions

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

In the equations above the x_3-axis is considered to be positive upward. 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:[2]

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

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

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

2.2 The estimation problem

We assume that the pressure head values p are recorded at the points x_{ri}, $1 \leq i \leq N_r$, inside Q for all $t \in I$. Then our objective is to use the observation vector $p^{obs}(t) = ((p(x_{ri}, t))_{1 \leq i \leq N_r}$ to infer the actual values of the permeability $k(x)$. We will consider the set of admissible parameters to be

$$\mathcal{P} = \{k : k \text{ is measurable}, \;\; k_* \leq k(x) \leq k^*\}$$

endowed with the $L^2(Q)$-topology.

We consider the cost functional $\mathcal{J}(k)$ defined as follows. For each point x_{ri} let B_i be a small ball of radius r small enough such that $B_i \cap B_j = \emptyset, i \neq j$. Then let us define

$$\begin{aligned} \widehat{p}(k, x_{ri}, t) = \frac{1}{|B_i|} \int_{B_i} p(k, x, t) dx, \\ \widehat{p}(k, t) = (p(k, x_{ri}, t))_{1 \leq i \leq N_r} \in R^{N_r}. \end{aligned} \tag{6}$$

Then let $\mathcal{J}(k)$ be defined by

$$\mathcal{J}(k) = \frac{1}{2}\|\widehat{p}(k) - p^{obs}\|_{L^2(I,R^{N_r})}. \tag{7}$$

Our estimation problem solved using a least squares criterion will be

$$\text{minimize} \quad \mathcal{J}(k) \quad \text{over} \quad \mathcal{P}. \tag{8}$$

2.3 The sensivity equations

The minimization problem requires the computation of the cost functional with respect to the parameter. We will denote by $D_k(p)\delta k$ the Gâteaux derivative of p in the direction of the perturbation δk of k. The Gâteaux derivative $D_k(p)\delta k$ can be computed as the solution of the following differential equation:

$$\begin{aligned} D_t(D_p(\theta)D_k(p)\delta k) - div(kg(p(k))D_xD_k(p)\delta k) - div((kD_p(g)D_k(p)\delta k)D_x(p + x_3)) = \\ div(g(p(k))\delta k D_x(p(k) + x_3)), \quad x \in Q,\ t \in I, \end{aligned} \tag{9}$$

with the boundary condition

$$-kg(p(k))D_xD_k(p)\delta k \cdot n = 0, \quad x \in \partial Q,\ t \in I, \tag{10}$$

and the initial condition

$$D_k(p)\delta k = 0, \quad t = 0, \quad x \in Q. \tag{11}$$

The functional $\mathcal{J}(k)$ has a Gâteaux derivative with respect to the parameter k given by

$$\mathcal{J}'(k)\delta k = \int_0^T \sum_{i=1}^{N_r} \left(\frac{1}{|B_i|} \int_{B_i} D_k(p)\delta k(x,t)\chi_{B_i}(x) \right) \left(\widehat{p}(k, x_{ri}, t) - p^{obs}(x_{ri}, t)\right) dt \tag{12}$$

where $\chi_{B_i}(x)$ denotes the characteristic function of the ball B_i.

The algorithm described in the next section is based on locating the zeros of $\mathcal{J}'(k)$.

3 THE ESTIMATION ALGORITHM

Using the above directional derivative we propose a Polak-Ribière conjugate gradient method to estimate the parameter $k(x)$.

From equation (12) it follows that the direction of steepest descent of $\mathcal{J}$ at the point $k_j(x)$ in the j-iteration is given by

$$d_j = D^*_{k_j}(p) \sum_{i=1}^{N_r} \frac{1}{|B_i|} \chi_{B_i}(x) \left(\widehat{p}(k_j, x_{ri}, t) - p^{obs}(x_{ri}, t)\right), \tag{13}$$

where $D_k^*(p)$ indicates the adjoint operator of $D_k(p)$.

The expression $D_k^*(p)\sum_{i=1}^{N_r}\dfrac{1}{|B_i|}\chi_{B_i}(x)\left(\widehat{p}(k,x_{ri},t)-p^{obs}(x_{ri},t)\right)$ has the representation:

$$D_k^*(p)(f) = -\int_0^T g(p(k))D_x(p(k)+x_3)\cdot D_xW(k)dt, \tag{14}$$

where $W(k)$ is the solution of the differential equation:

$$\begin{aligned} -D_p(\theta)D_tW(k) - div(kg(p(k))D_xW(k)) \\ +kD_p(g)D_x(p(k)+x_3)\cdot D_xW(k) = f, \quad x\in Q,\ t\in I, \end{aligned} \tag{15}$$

with boundary conditions

$$kg(p(k))D_xW(k)\cdot n = 0 \quad x\in\partial Q,\ t\in I,, \tag{16}$$

and final condition

$$W(k)(\cdot,T) = 0, \quad x\in Q. \tag{17}$$

The function f is the residual-related function given by

$$f(x,t) = \sum_{i=1}^{N_r}\frac{1}{|B_i|}\chi_{B_i}(x)\left(\widehat{p}(k,x_{ri},t)-p^{obs}(x_{ri},t)\right). \tag{18}$$

Then, a minimization procedure using a Polak-Ribière conjugate gradient iteration can be stated as follows:

- 1) Give an initial guess $k_0(x)$, compute $p(k_0)$ by solving (1)-(3).
- 2) Compute the direction of steepest descent d_0 using (13).
- 3) Set $j=0$.
- 4) Compute the descending step length α_j

  $$\alpha_j = -\frac{\int_0^T\sum_{i=1}^{N_r}\left(D_{k_j}(p)d_j\right)\left(p-p^{obs}\right)(x_{ri},t)dt}{\int_0^T\sum_{i=1}^{N_r}\left(D_{k_j}(p)d_j(x_{ri},t)\right)^2 dt}$$

  where $D_{k_j}(p)d_j$ is the solution of (9) for the choice $\delta k = d_j$.
- 5) Update the saturated hydraulic conductivity as follows:

  $$k_{j+1} = k_j + \alpha_j d_j.$$

- 6) Compute $p(k_{j+1})$ by solving (1)-(3).

- 7) Compute error, if convergence is achieved, stop.
- 8) Compute $\mathcal{J}'(k_{j+1})$ using (12).
- 9) Compute β_{j+1} using the Polak-Ribière formula[22]

$$\beta_{j+1}^{PR} = \frac{\| \mathcal{J}'(k_{j+1}) \left(\mathcal{J}'(k_{j+1}) - \mathcal{J}'(k_j) \right) \|_{L^2(Q)}}{\| \mathcal{J}'(k_j) \|^2_{L^2(Q)}}$$

- 10) Compute the search direction

$$d_{j+1} = -\mathcal{J}'(k_{j+1}) + \beta_{j+1}^{PR} d_j.$$

- 11) New iteration: set $j = j + 1$ and go to 4).

Also, for improving the convergence of the Polak-Ribière conjugate gradient method a restart procedure was implemented as described in.[23] The numerical solutions of the direct problem (1)-(3), the Gâteaux derivatives (9)-(11) and the adjoint problem (15)-(17) were obtained using Galerkin finite element procedures.

4 NUMERICAL EXPERIMENTS

The proposed algorithm was implemented to estimate the saturated permeability $k(x)$ in a vertical heterogeneous soil profile during an infiltration 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 250 cm soil profile Q consisting of six layers with the following values of saturated permeability

$$k(x) = \begin{cases} 4.5\ 10^{-3} \text{ cm/s} & 0 \text{ cm} \leq x < 45 \text{ cm} \\ 4.0\ 10^{-3} \text{ cm/s} & 45 \text{ cm} \leq x < 85 \text{ cm} \\ 5.0\ 10^{-3} \text{ cm/s} & 85 \text{ cm} \leq x < 125 \text{ cm} \\ 6.0\ 10^{-3} \text{ cm/s} & 125 \text{ cm} \leq x < 165 \text{ cm} \\ 5.0\ 10^{-3} \text{ cm/s} & 165 \text{ cm} \leq x < 205 \text{ cm} \\ 5.5\ 10^{-3} \text{ cm/s} & 205 \text{ cm} \leq x \leq 250 \text{ cm.} \end{cases} \tag{19}$$

The other hydraulic parameters of van Genuchten model are arbitrarily assumed to be constant over the whole profile with θ_s = 0.368, θ_r = 0.104, n = 2.0 and α_{vg} = 0.0335 cm^{-1}.

In the infiltration experiment, water is uniformly applied on the soil surface ($x = 250$ cm) at a rate of $2.5\ 10^{-5}$ cm/s for a period of 9 days. The initial pressure head of the soil profile was assumed to be constant and equal to -400 cm. The numerical test is stopped when the infiltration front reaches the bottom boundary where a no-flux condition is prescribed. The time step used in the numerical solution of Richard's equation, the Gâteaux derivative and the adjoint problem is $\Delta t = 864$ s with a uniform partition $\mathcal{T}^h$ of Q into elements Q_j of size $h = 2.77$ cm.

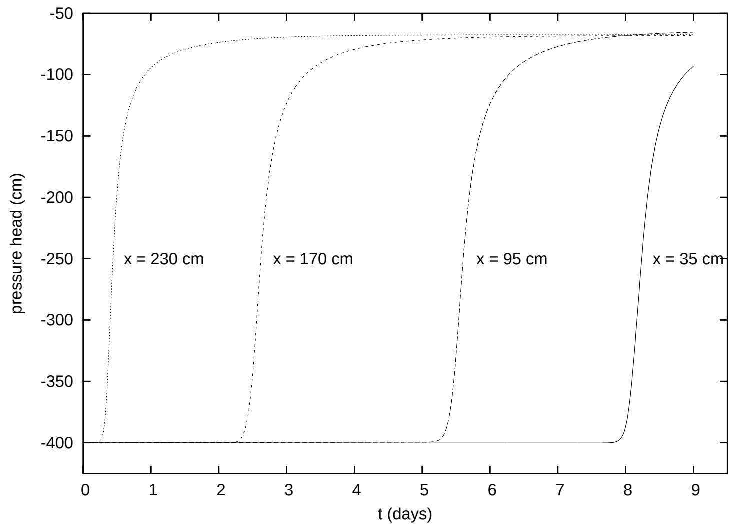

Figure 1: Simulated pressure head observations at $x = 35, 95, 170$ and 230 cm depths.

The pressure head values were assumed to be recorded at discrete times t_n at 16 points x_{ri} spaced 15 cm from each other. Figure 1 shows simulated pressure head observations at the recording points x = 35 cm, 95 cm, 170 cm and 230 cm.

The initial guess for $k(x)$ in the inverse procedure was taken to be constant an equal to $5.0\ 10^{-3}$ cm/s. Figure 2 shows the initial guess and the updates profiles of $k(x)$ after 10 and 50 iterations, where some oscillations in the estimated profiles can be observed. To eliminate these oscillations and stabilize the parameter estimation procedure a simply postprocessing algorithm of the predicted $k(x)$ profile was implemented. At each element Q_j the saturated permeability value was updated using a weighted average of its values at neighboring elements.

Figure 3 shows the updated profiles of $k(x)$ after 100, 300 and 500 iterations. Numerical oscillations almost disappear after 100 iterations and the estimate profile is quite accurate except near the domain boundaries where convergence is slow. Note that in this numerical example the permeability values are not assumed to be known near the top surface as it was assumed in the derivation of our estimation procedure. The algorithm first quickly reached the true permeability values in the interior of the domain and then slowly adjusted the true permeability profile near the surface and bottom boundaries.

5 CONCLUSIONS

An iterative algorithm to estimate the saturated hydraulic conductivity in one-dimensional layered unsaturated soils is presented. The inverse problem is posed as a functional optimization problem and the gradient of the cost functional was computed by solving the associate adjoint problem. This allows for the formulation of the conjugate gradient algorithm to solve the estimation 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

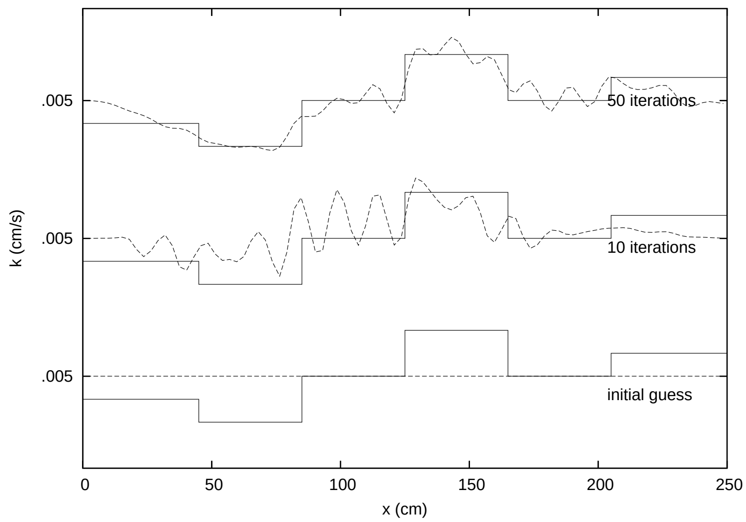

Figure 2: Initial, estimated (dashed) and true (continuous) saturated permeability.

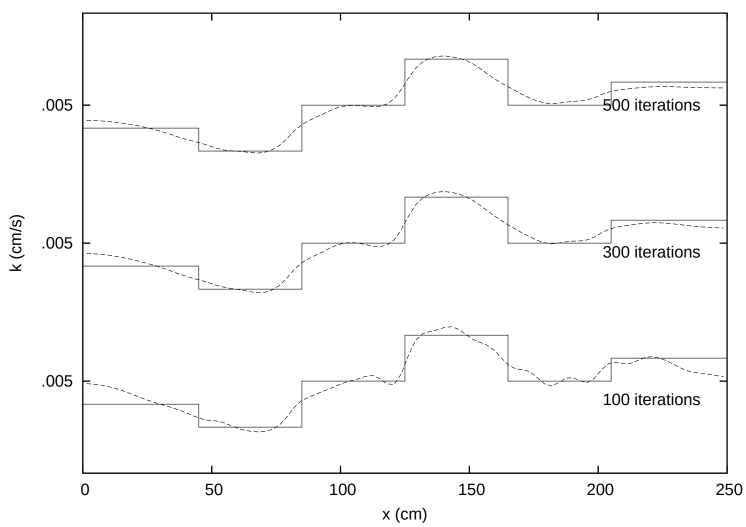

Figure 3: Estimated (dashed) and true (continuous) saturated permeability.

the direct and the adjoint problems and the Gâteaux derivatives. From the numerical example shown in Section 4, we can conclude that the proposed algorithm yields a very good estimate of saturated permeability in a stratified medium and becomes a promising method for *in situ* estimation of this parameter under unsaturated conditions.

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