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An Inverse Problem Approach for the Optimization of the Haverkamp and van Genuchten Retention Curves Parameters with the Luus-Jaakola Method

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1 Introduction

The movement of water in the soil is an important process in studies of management and conservation of water resources, irrigation and drainage, as well as in the transport of solutes (nutrients and pesticides). The water transport in the soil can be described numerically using Richards equation, which combines Darcy's law and the continuity equation. However, for its solution, it is necessary to know the relationship between soil water content and pressure head, described by a water retention curve. The water retention curve can be represented by several empirical models, in which their coefficients must be fitted to different soil types. The determination of the coefficients using traditional methods (e.g. Richards pressure plate apparatus) demands a significant amount of time and financial resources. Thus, the present article proposes the use of inverse modeling techniques to fit the coefficients of the soil water retention curve. In this way, the problem of inverse modeling is solved by means of the squared residues functional minimization [8]. In the present work, we use the Luus-Jaakola method [7, 10], a stochastic method, in the determination of the parameters of interest.

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2 Mathematical Model

Consider the values obtained experimentally for the soil water content, θ_e. The residue between the calculated, θ_c, and experimental quantity is given by

$$\mathbf{R} = \theta_c - \theta_e \tag{1}$$

where the subscript c indicates the value of θ calculated computationally, and the subscript e indicates the value of θ obtained experimentally in the field, θ ($m^3\,m^{-3}$). The objective is that the residue be as small as possible. Then, there is a minimization problem to be tackled.

The functional of square residuaes is given by

$$Q(\mathbf{P}) = \frac{1}{2}|\mathbf{R}|^2 = \frac{1}{2}\mathbf{R}^T\mathbf{R} \tag{2}$$

where $\mathbf{R} = (R_1, ..., R_M)^T \in I\!R^M$ represents the vector of residues, M is the amount of experimental data, and $\mathbf{P}$ represents the parameters to be estimated, or, in other words, the solution of the inverse problem [8].

Replacing (1) in (2), results

$$Q(\mathbf{P}) = \frac{1}{2}\sum_{i=1}^{M}(\theta_{c_i} - \theta_{e_i})^2 \tag{3}$$

2.1 Richards' One-Dimensional Equation

In order to solve water infiltration problems in soil, the Richards equation, described in its ψ-based form, is given by

$$C(\psi)\frac{\partial\psi}{\partial t} = \frac{\partial}{\partial z}\left[K(\psi)\frac{\partial\,(\psi - z)}{\partial z}\right] \tag{4}$$

where ψ is the pressure head (cm), $C(\psi)$ is the water capacity, t is the time, $K(\psi)$ is the hydraulic conductivity ($cm\,d^{-1}$), and z is the vertical coordinate (cm), from the origin to the negative axis, $-z$ [2, 9, 11]. The initial condition and the boundary conditions will be defined in the section 4.

The equation for modeling the retention curve has already been proposed by several authors [2]. In this work the curves of van Genuchten (eq. 5) [1] and of Haverkamp (eq. 6) [4] were chosen. They relate the soil water content and pressure head, $\theta = \theta(\psi)$, and are given, respectively, by

$$\theta(\psi) = \theta_r + (\theta_s - \theta_r)\,(1 + |\alpha\psi|^n)^{-m} \tag{5}$$

$$\theta(\psi) = \theta_r + \frac{B(\theta_s - \theta_r)}{B + |\psi|^\lambda} \tag{6}$$

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The equations of hydraulic conductivity of van Genuchten (eq. 7) and of Haverkamp (eq. 8) are given by

$$K(\psi) = K_s \left(1 - (\alpha|\psi|)^{n-1} \left[1 + (\alpha|\psi|)^n\right]^{-m}\right)^2 \left[1 + (\alpha|\psi|)^n\right]^{-m/2} \tag{7}$$

$$K(\psi) = K_s \cdot \frac{A}{A + |\psi|^{\phi}} \tag{8}$$

In equations (5) to (8), we have that θ_s is the saturated water content (cm^3cm^{-3}), θ_r is the residual water content after drying the soil (cm^3cm^{-3}), K_s is the hydraulic conductivity saturated ($cm\,d^{-1}$), and α (cm^{-1}), n and m (dimensionless) are empirical factors. The parameters m and n are related by $m = 1-1/n$, [6]. In equations (6) and (8) λ is an index related to the distribution of soil pores (cm), A, B and ϕ are dimensionless parameters.

2.2 Direct Problem Solution

According to Guterres [2], in regard to solving flow problems in porous media, a fundamental characteristic sought is the observance of mass conservation, an essential requirement for the solution to have physical meaning. Then, since the conservation of the physical quantities at the discrete level is an intrinsic feature of the Finite Volume Method (FVM), this method was implemented to solve the Richards equation [9].

3 Inverse Problem Solution

Luus and Jaakola [7, 10] developed a simple optimization procedure to solve nonlinear programming problems. The procedure is based on minimizing the functional given by equation (3). For that purpose, restrictions are defined as

$$MIN_{\mathbf{P}} < \mathbf{P} < MAX_{\mathbf{P}} \tag{9}$$

where $MIN_{\mathbf{P}}$ and $MAX_{\mathbf{P}}$ are respectively the vectors containing the lower and upper limits of the search interval for the parameters of interest (vector $\mathbf{P}$), and $\#(\mathbf{P})$ is the number of parameters to be estimated.

This is a conditional minimization problem. The Luus-Jaakola's proposal is described in the algorithm below.

1. Read the vector with experimental data θ_e.
2. The restrictions are defined, ie, the maximum value and the minimum value for $\mathbf{P}$, see equation (9), according to the existing literature.
3. An initial random estimate (candidate solution) is generated, within the constraints described in the previous step. Denote these initial values as $\mathbf{P}^0$, and the amplitude of the search interval $\mathbf{r}^0 = MAX_{\mathbf{P}^0} - MIN_{\mathbf{P}^0}$;
4. Solve Richard's equation, i.e. equation (4), and calculate the residue $Q_0 = Q(\mathbf{P}^0)$ according to equation (3);

5. Define the number of times that the amplitude of the search interval is reduced. Denote this amount by N_{out}.
6. Define a number of possible candidate solutions, N_{int}.
7. For $i = 1 : N_{out}$ do:
   (a) For $j = 1 : N_{int}$ do:
      i. Generate random numbers between -0.5 e $+0.5$ for each of the parameters to he determined. Denote these by $\mathbf{Y}$;
      ii. Take random numbers from step (7(a)i) and attribute to the new candidate solution $\mathbf{P}$, $\mathbf{P}^{new}$, given by
$$P_k^{i,j} = P_k^{i-1,j} + Y_k \cdot r_k^{i-1} \quad , \quad k = 1, \ldots, \#(\mathbf{P})$$
      iii. Test the restrictions imposed for each P_k, $i = 1, \ldots, \#(\mathbf{P})$. If $P_k > MAX_{P_k}$, then do $P_k = MAX_{P_k}$. Se $P_k < MIN_{P_k}$, then do $P_k = MIN_{P_k}$;
      iv. Calculate the new value θ_c, using equation (4);
      v. Calculate the new residue $Q_{new} = Q(\mathbf{P}^{new})$ according to equation (3);
      vi. If $Q_{new} < Q_0$, then assume the new parameters obtained at random as the optimal solution of the problem and $Q_0 = Q_{new}$. Otherwise, discard the new values for $\mathbf{P}$;
   (b) If i did not reach N_{out}, reduce the amplitude of the search interval by a percentage pre-defined in the algorithm, called ϵ, $\mathbf{r}^i = (1-\epsilon)\mathbf{r}^{i-1} \quad 0 < \epsilon < 1$;
8. At the end of the procedure $\mathbf{P}$ is the best candidate solution which minimizes the functional $Q(\mathbf{P})$.

4 Results

The numerical results obtained are presented next. As described prevously, the direct problem was solved using the FVM, and the Inverse Problem with the Luus-Jaakola's method. Both algorithms were implemented using SciLab, a free software developed for scientific work research.

4.1 Test case 01 - van Genuchten

In this case it is considered a depth, $Lz = 60\,cm$, time of $1200\,s$, and conditions of the Dirichlet type. The conditions are described below.

$$\begin{cases} \psi(z,0) &= -350.0\ cm, 0 < z < Lz \\ \psi(0,t) &= -10.0\ cm, t > 0 \\ \psi(L_z,t) &= -350.0\ cm, t > 0 \end{cases} \tag{10}$$

Consider the values of the parameters of the problem, $K_s = 6.2611 \times 10^{-3}$, $\alpha = 2.80 \times 10^{-2}$, $n = 2.239$, $m = 0.5534$, $\theta_r = 0.029$ and $\theta_s = 0.366$.

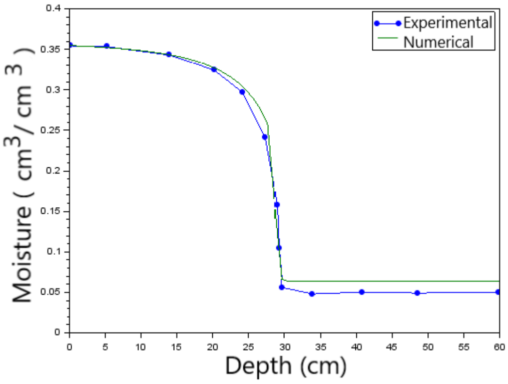

Figure 1: Solution for the soil moisture content with $N_{out} = 150$, $N_{int} = 50$ and $\epsilon = 0.2$, in the Luus-Jaakola method considering van Genuchten's retention curve.

The values of the parameters obtained with the iterative procedure for the solution of the inverse problem were $\alpha = 2.68748 \times 10^{-2}$, $n = 2.0140123$ and $m = 0.5034787$, see Table 1. Statistical data that measures the accuracy and precision of the model are $r^2 = 0.989$ and $d = 0.997$, very close to the ideal value 1, and the square root of the residue was 0.0521, [12]. Figure 1 shows the soil moisture content based on the parameters obtained by the Luus-Jaakola method for the van Genuchten retention curve.

Table 1: Parameters of the van Genuchten's retention curve.

	α	n	m
van Genuchten parameters	2.80×10^{-2}	2.239	0.5534
LJ parameters	2.68748×10^{-2}	2.0140123	0.5034787

4.2 Test case 02 - Haverkamp

In this case it is considered a depth, $Lz = 100\,cm$, time of $0.8\,h$, and conditions of the Dirichlet type. The conditions are described below.

$$\begin{cases} \psi(z,0) &= -61.50\ cm, 0 < z < Lz \\ \psi(0,t) &= -20.73\ cm, t > 0 \\ \psi(L_z,t) &= -61.50\ cm, t > 0 \end{cases} \tag{11}$$

Consider the values of the parameters of the problem, $K_s = 9.44 \times 10^{-3}$, $A = 1.19 \times 10^6$, $\phi = 4.74$, $B = 1.611 \times 10^6$, $\lambda = 3.96$, $\theta_r = 0.075$ and $\theta_s = 0.287$.

The inverse problem was solved to obtain four parameters: A, B, λ and ϕ. Simulations were performed with various values for N_{out} and N_{int}. The best configuration was for $N_{out} = 200$ and $N_{int} = 25$. Figure 2 shows the soil moisture content based on the parameters obtained by the Luus-Jaakola method, see Table 2, for Haverkamp's retention

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curve. Good results were obtained, whose statistical indixes are $r^2 = 0.995$ and $d = 0.990$, [12].

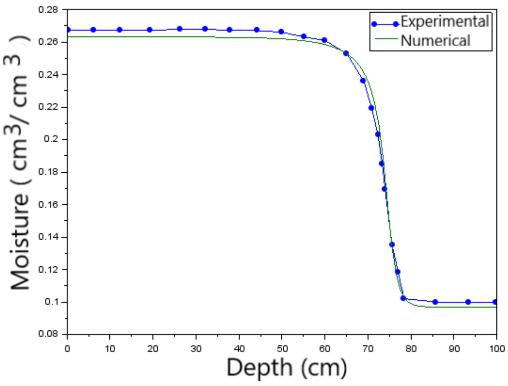

Figure 2: Solution for the soil moisture content with $N_{out} = 200$, $N_{int} = 25$ and $\epsilon = 0.2$, in the Luus-Jaakola Method, considering Haverkamp's retention curve.

Table 2: Parameters of the Haverkamp's retention curve.

	B	λ	A	ϕ
Haverkamp parameters	1.611×10^6	3.96	1.19×10^6	4.74
LJ parameters	1.141×10^6	3.93	1.98×10^6	4.92

5 Conclusions

The Luus-Jaakola's method yielded good results, as can be observed in the statistical data presented, as well as in the moisture content profiles. Being the Luus-Jaakola a probabilistic method, there is always the possibility of not returning the expected values, as happened with test cases with small values for N_{out} and N_{int}. As future work it will be considered the implementation of the modified Luus-Jaakola's method, [5], in order to compare the error and reduce the computational time.

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References

[1] M. T. van Genuchten, A closed-form equation for predicting the hydraulic conductivity of unsaturated soils, *Soil Science Society of America Journal*, 44:5:892–898, 1980.

[2] M. X. Guterres, Evaluation of the Picard-Krylov and Newton-Krylov algorithms in the solution of the Richards equation, Tese de doutorado, IPRJ/UERJ, 2014 (In Portuguese).

[3] M. X. Guterres and J. F. V. Vasconcellos and A. J. Silva-Neto and C. B. L. Peralta and L. G. M. F. Teixeira. Approximation of a Solution for the Richards 2D Equation by the Finite Volume Method with the Aid of the Picard-Krylov Algorithms (In Portuguese), Águas Subterrâneas, Volume 31:2:89-108, 2017.

[4] R. Haverkamp and M. Vauclin and J. Touma and P. J. Wierenga and G. Vachaud. A comparison of numerical simulation models for one-dimensional infiltration, *Soil Science Society of America Journal*, volume 41:2:285-294, 1977.

[5] J. Jezȯowski and R. Bochenek and G. Ziomek. Random Search Optimization Approach for Highly Multi-Modal Nonlinear Problems. Advances in Engineering Software 36, 504-517, 2005.

[6] J. G. Kroes and J. C. van Dam and P. Groenendijk and R. F. A. Hendriks and C. M. J. Jacobs. SWAP version 3.2. Theory description and user manual, *Wageningen, Alterra, Alterra Report 1649(02)*, 2008. ISSN 1566-7197.

[7] R. Luus and T. H. I. Jaakola. Optimization by Direct Search and Systematic Reduction of the Size of Search Region, *AIChE Journal*, volume 19:4:760-766, Toronto, Canadá, 1973.

[8] F. D. Moura-Neto and A. J. Silva-Neto. An Introduction to Inverse Problems with Applications. Springer-Verlag, 2012.

[9] M. O. Temperini,Inverse modeling to obtain parameters for Richards equation (in Portuguese), Dissertação de Mestrado, PGEB/UFF, 2018.

[10] A. J. Silva-Neto and J. C. Becceneri and H. F. Campos Velho. Computational Intelligence Applied to Reverse Problems in Radiative Transfer (In Portuguese), EdUERJ, 2016. ISBN 978-85-7511-368-4.

[11] A. J. Silva Neto and R. E. White. Numerical Solution of Fluid in Partially Saturated Porous Media, Transactions of the Eleventh Army Conference on Applied Mathematics and Computing, ARO Report 94-1, Carnegie Mellon University, June 8-10. pp. 353-371, 1994.

[12] C. J. Willmott. On the validation of models. Physical Geography, volume 2:2., USA, 2013.

