25th ABCM International Congress of Mechanical Engineering
October 20-25, 2019, Uberlândia, MG, Brazil

COBEM2019-1110
COMPARISON OF VARIANTS OF THE LUUS-JAAKOLA METHOD IN THE ESTIMATION OF VAN GENUCHTEN RETENTION CURVE PARAMETERS

Fábio Freitas Ferreira
Wagner Rambaldi Telles
Universidade Federal Fluminense
fabiofreitasferreira@id.uff.br
wr_telles@yahoo.com.br

Gustavo Bastos Lyra
Universidade Federal Rural do Rio de Janeiro
bglyra@id.uff.br

Antônio J. Silva Neto
Universidade do Estado do Rio de Janeiro
ajsneto@iprj.uerj.br

Abstract. *In order to predict volumetric water content, it is necessary to know the water retention curve in the soil, as well as the hydraulic conductivity function. These functions depend on parameters related to the soil physical characteristic such as texture. It is in this sense that the aim of this work is to compare the three versions of the Luus-Jaakola method.*

Keywords: *Inverse Problem, Luus-Jaakola, Richards Equation, van Genuchten, Retention Curves*

1. INTRODUCTION

Inverse problems are of great importance in several relevant real world applications, and has attracted the attention of an increasing number of researchers. Many processes that usually require high financial costs, or time, can be improved with the application of optimization methods. Problems of infiltration of water into soil are of particular interest for enviromental modelling and food production, among many other applications. These problems depend on parameters that need to be obtained through specific equipment, which depends on the soil characteristic. To prescribe the infiltration of water into the soil, the Richards equation has been intensively used in Silva Neto and White (1994) and Kroes *et al.* (2017). This equation is a combination of the Darcy equation and the continuity equation, which depends on the water retention curve in the soil, as well as the hydraulic conductivity function. This problem has been treated over the decades, as can be seen in Silva Neto and White (1994) and Celia *et al.* (1990). In Temperini (2018) we find the solution of the Richards Equation by means of the Finite Volume Method (FVM).

In Moura Neto and Silva Neto (2012), we find a description of inverse problems, and solution methods known as deterministic methods. Another class of inverse problems solution approach is related to stochastic methods. In Telles (2014) and in Silva Neto *et al.* (2016), we find the application of the Luus-Jaakola method, a probabilistic, easy-to-implement method that was developed to solve problems of maximization and minimization.

Jezȯwski *et al.* (2005) proposed two modifications in the Luus-Jaakola method. Both changes involves the strategy for the reduction of the search interval. It is in this sense that the aim of this work is to apply such modifications to the problem of infiltration of water in the soil, specifically the estimation of the van Genunchten retention curve parameters, and compare the solution with the original LJ.

2. MATHEMATICAL MODEL

Let θ_e be the soil volumetric water content (cm^3/cm^3), obtained experimentally in a soil column, and θ_c be the soil volumetric water content (cm^3/cm^3) obtained by means of the algorithm developed by Temperini (2018), using the FVM. The residue between the experimental and the calculated values is given by $\mathbf{R} = \theta_c - \theta_e$. We define the functional that represents the summation of squared residuals by

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

where $\mathbf{R} = (R_1, ..., R_M)^T \in I\!R^M$ is the vector containing the residues, M is the amount of experimental data, and $\mathbf{P}$ represents the parameters to be estimated. According the definition by Silva Neto and Moura Neto (2005), this is a type 2 problem.

The functional (1) can be rewritten as

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

2.1 DIRECT PROBLEM

In Temperini (2018), Kroes *et al.* (2017), Guterres (2013) and Guterres *et al.* (2017), the soil water infiltration problem is modelled with Richards equation. In Temperini (2018), it is obtained the solution of the ψ-based form using the Finite Volume Method (FVM), employing the van Genuchten and Haverkamp retention curves, which is given by

$$C(\psi)\frac{\partial \psi}{\partial t} = \frac{\partial}{\partial z}\left[K(\psi)\frac{\partial\left(\psi - z\right)}{\partial z}\right] \tag{3}$$

where ψ is the pressure head (cm), $C(\psi)$ is the water capacity, $C(\psi) = \partial\theta/\partial\psi$, 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, $-z$, as defined in Guterres (2013), Temperini (2018), and Silva Neto and White (1994).

In the present work, we consider the soil water retention curve proposed by van Genuchten, $\theta = \theta(\psi)$, and hydraulic conductivity, $K(\psi)$, which are given by

$$\theta(\psi) = \theta_r + (\theta_s - \theta_r)\left(1 + |\alpha\psi|^n\right)^{-m} \tag{4}$$

and

$$K(\psi) = K_s\left(1 - (\alpha|\psi|)^{n-1}\left[1 + (\alpha|\psi|)^n\right]^{-m}\right)^2\left[1 + (\alpha|\psi|)^n\right]^{-m/2} \tag{5}$$

where θ_s is volumetric water content of the saturated soil $(cm^3 cm^{-3})$, θ_r the volumetric water content of the residual soil, that is, after soil drainage $(cm^3 cm^{-3})$, K_s is the hydraulic conductivity saturated $(cm\, d^{-1})$, and α (cm^{-1}), n and m (dimensionless) are empirical factors. The parameter m is related to the parameter n acoording to the relation $m = 1 - 1/n$.

The study on the estimation of the parameters θ_s, θ_r, α and n is the main objective of this work, that is, the solution of the inverse problem for the estimation of the vector of parameters $\mathbf{P} = (\alpha, n, \theta_r, \theta_s)$.

2.2 SENSITIVITY ANALYSIS

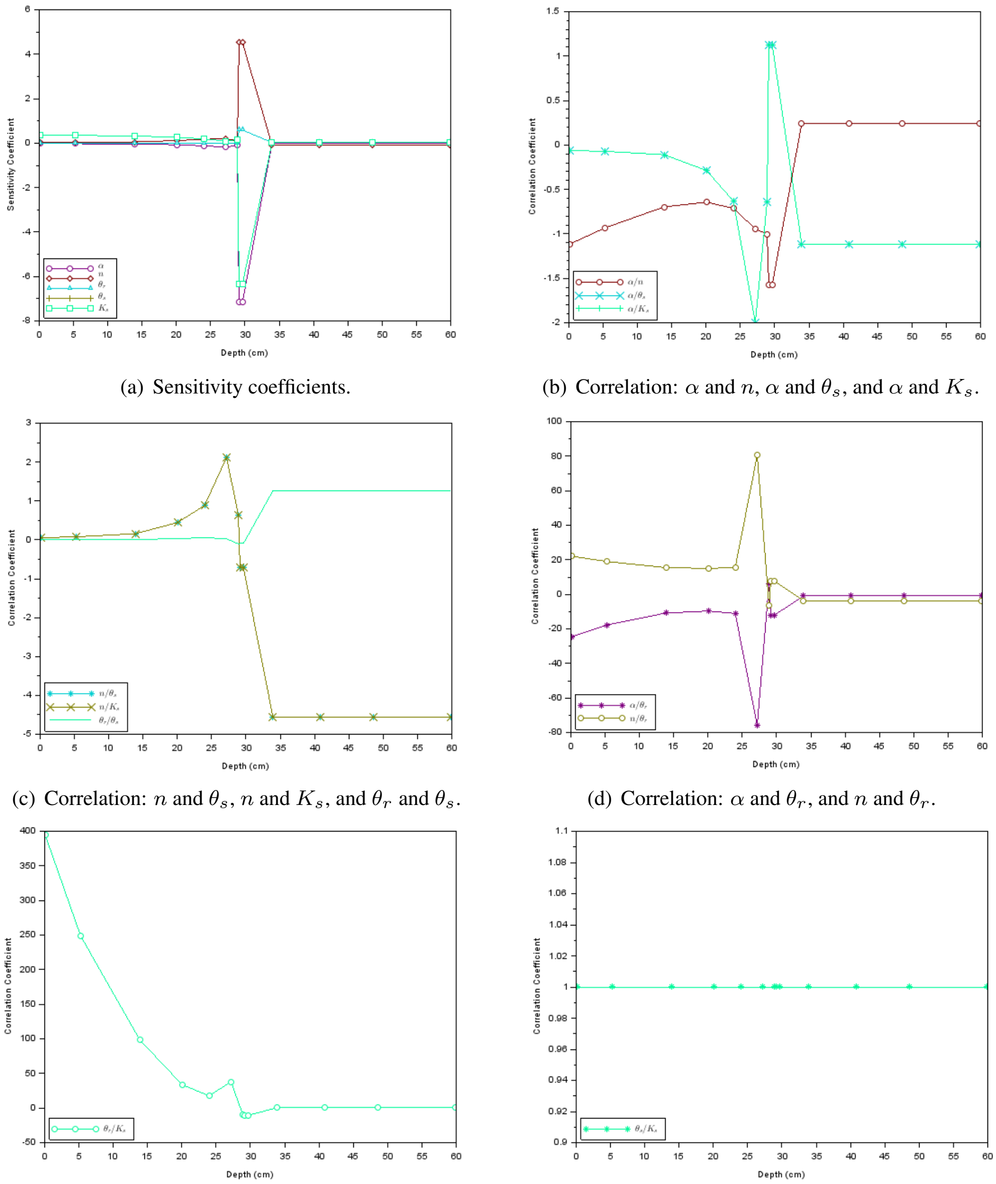
In this section we present the problem sensitivity analysis for the case presented in the section 3. This analysis allows us to pre-understand the behavior of some parameters, thus making some decisions about which parameters to determine.

Sensitivity coefficients are given by

$$X_i = \frac{\partial\theta}{\partial\Delta\mathbf{P}_i} \quad i = 1:N \tag{6}$$

where N is the total of problem parameters.

Sensitivity coefficients are not expected to be null, as we know that two distinct parameter sets, $\mathbf{P}$ and $\mathbf{P} + \Delta\mathbf{P}$, will return $\theta(\mathbf{P}) \neq \theta(\mathbf{P} + \Delta\mathbf{P})$. It can be seen in Figure 1(a) the sensitivity coefficients. Changes occur between the depths 20cm and 35cm, where the retention curve varies from asymptote θ_s until the asymptote θ_r. All parameters showed good sensitivity coefficients. Another analysis made is the correlation between the parameters. The Figure 1(f) shows a linear dependence between the parameters θ_s and K_s. This shows that these two parameters can not be obtained simultaneously. Because it is a problem of water infiltration in the soil, this analysis varies from case to case, because there are different types of soils and parameter values can change dramatically in a clay soil to a sandy soil.



(a) Sensitivity coefficients.

(b) Correlation: α and n, α and θ_s, and α and K_s.

(c) Correlation: n and θ_s, n and K_s, and θ_r and θ_s.

(d) Correlation: α and θ_r, and n and θ_r.

(e) Correlation: θ_r and K_s

(f) Correlation: θ_s and K_s

Figure 1. Sensitivity analysis of van Genuchten parameters.

2.3 INVERSE PROBLEM

The method of Luus and Jaakola (1973), was developed for optimization problems of nonlinear programming. The procedure aims at minimizing a functional, in this case given in equation (2). In a constrained minimization problem it is necessary to define the constraints, given by

$$MIN_{\mathbf{P}} < \mathbf{P} < MAX_{\mathbf{P}} \tag{7}$$

where $\mathbf{P}$ is the vector that contains the parameters to be estimated.

The algorithm for solving the problem is presented in the flowchart in Figure 2. In the algorithm $NOUT$ is the number of times that the amplitude of the search interval is reduced, $NINT$ is the quantity of possible candidates for solution, $FitnessOld$ always keeps the smallest residue between the experimental data and the solution obtained with the direct problem, $Fitness$ saves the residue at each iteration of the algorithm, and $count$ is the counter of iterations.

In the original LJ, the amplitude of the search interval is reduced along the iterative procedure using $r = (1-\epsilon)r, \quad 0 < \epsilon < 1$, wherein ϵ is a predefined reduction factor, and the initial search interval is defined by $\mathbf{r} = MAX_{\mathbf{P}} - MIN_{\mathbf{P}}$. In the modified method LJ-MM Version 1, $\epsilon = 0.001/[(MAX - MIN)^{1/NOUT}]$ and $r = r \cdot \epsilon$. In the modified method LJ-MM Version 2, ϵ is reset to each $NOUT$, ie, $\epsilon = 0.001/[(MAX - MIN)^{k/NOUT}]$, $k = 1, \ldots, NOUT$ and $r = (MAX - MIN) \cdot \epsilon$.

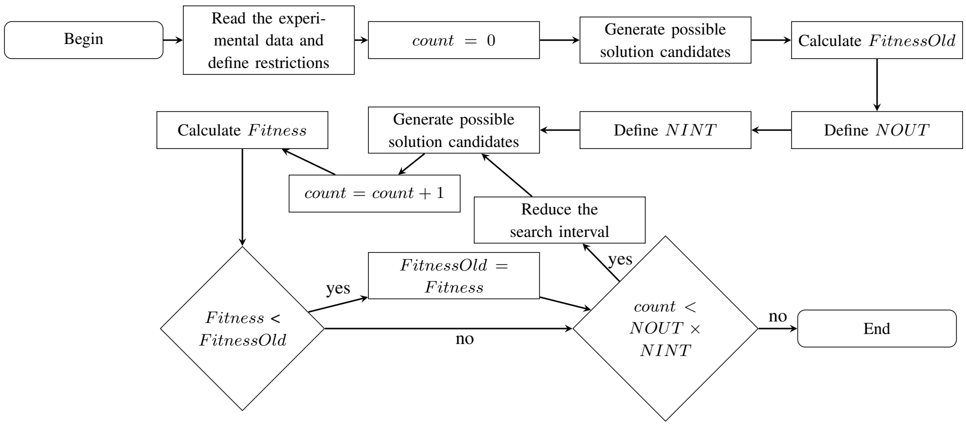


Figure 2. LJ Method Flowchart

3. RESULTS AND DISCUSSION

In order to test the three versions of the LJ Method, the original and the two modified ones, it was considered the test case presented in de Vasconcellos and Amorim (2001). Here it is used a soil depth of $60\,cm$, $Lz = 60\,cm$, simulation time of $1200\,s$, and boundary conditions of the Dirichlet type, $\psi(0,t) = -10.0\ cm$, $t > 0$, and $\psi(L_z,t) = -350.0\ cm$, $t > 0$, and the initial condition $\psi(z,0) = -350.0\ cm$, $0 \leq z \leq Lz$.

The original parameters of the van Genuchten retention curve, equation (4), are $\alpha = 2.80 \times 10^{-2}\ cm^{-1}$, $n = 2.239$, $\theta_r = 0.029\ cm^3cm^{-3}$ and $\theta_s = 0.366\ cm^3cm^{-3}$.

First, all parameters were simulated, except m which can be obtained by the relation $m = 1 - 1/n$. The restrictions have to limit the parameters within an initial search interval is was used $0 \leq \alpha \leq 1,\ 0.1 \leq n \leq 6,\ 0.01 \leq \theta_r \leq 0.1$ and $0.1 \leq \theta_s \leq 0.5$.

In the Table 1 all results obtained with the three versions of the LJ method are presented. Subsequently, a statistical analysis of these results is made.

Table 1. Parameters obtained for the three versions of LJ in the ten rounds.

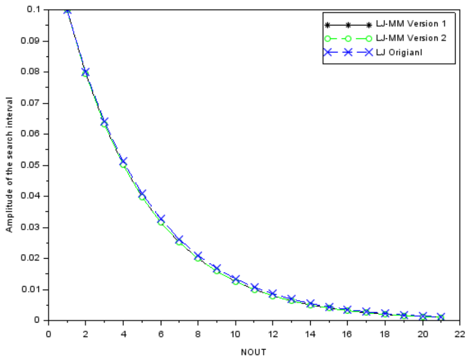
	LJ0				LJ version 1				LJ version 2			
Rodada	α	n	θ_r	θ_s	α	n	θ_r	θ_s	α	n	θ_r	θ_s
1	0.0318	2.2592	0.0185	0.3072	0.0497	1.6025	0.0998	0.3985	0.0143	1.7139	0.0494	0.2265
2	0.0333	1.6799	0.0668	0.3206	0.0464	2.0794	0.0586	0.2512	0.1000	1.2486	0.0100	0.5000
3	0.0441	1.9711	0.1000	0.3139	0.0377	1.9595	0.0672	0.3822	0.0083	2.7658	0.1000	0.4757
4	0.0236	1.8115	0.0506	0.3705	0.0235	1.7961	0.0592	0.324	0.0700	1.7832	0.1000	0.4073
5	0.0352	2.2087	0.0742	0.3955	0.0371	3.0000	0.0844	0.2866	0.0186	1.9957	0.1000	0.3619
6	0.0241	1.5317	0.0644	0.3944	0.0489	2.5247	0.0969	0.3002	0.0119	3.0000	0.0558	0.2546
7	0.0305	2.2053	0.0100	0.3189	0.0133	3.0000	0.0993	0.2114	0.0125	1.5068	0.0990	0.2301
8	0.0326	2.9945	0.0100	0.2607	0.0416	1.6245	0.0346	0.3858	0.0109	3.0000	0.0687	0.3273
9	0.0450	2.3408	0.0845	0.3084	0.0308	1.9860	0.0236	0.4053	0.0348	1.6316	0.0119	0.3565
10	0.0386	3.0000	0.1000	0.3129	0.0483	2.0582	0.0978	0.2873	0.0734	1.4461	0.0658	0.2131

In a first analysis showed the amplitude of the search interval, r. In Figures 4(a) and 4(c) have the LJ Original, with $\epsilon = 0.2$, is smooth by reducing the amplitude of the search interval. In the LJ-MM Version 1 and LJ-MM Version 2, there is a very rapid reduction in relation to the parameters n and θ_s, making possible solution candidates to be left out of the search.

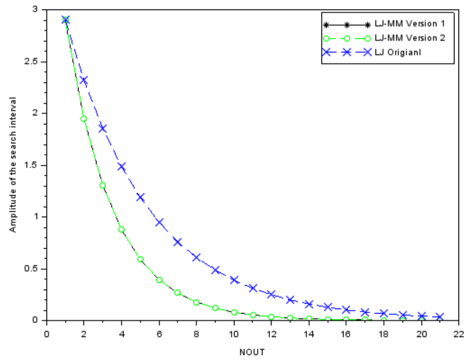
In Figure 4, we observe the standard deviation considering the 10 runs of each method. In both cases the dispersion is smaller for the original LJ. Observing the behavior of FitnessOld, one realizes this fact. No caso dos parâmetros α, n e θ_s, for the original LJ, FitnessOld is reduced along the search. Already in LJ version 1 and version 2, FitnessOld arrives there is a minimum value, just after count reaches 100, that the algorithm can not get out.

In Figure 5 it is observed that the best results were obtained with the settings where $NINT > 50$, as shown in Figure 5. The behavior of the function was recovered with the original LJ. The LJ-MM version 1 and LJ-MM version 2 can not recover the same behavior. In the original LJ, the solution is improved as the NOUT is increased. In the LJ-MM the ideal solution is obtained with a maximum of NOUT = 3.

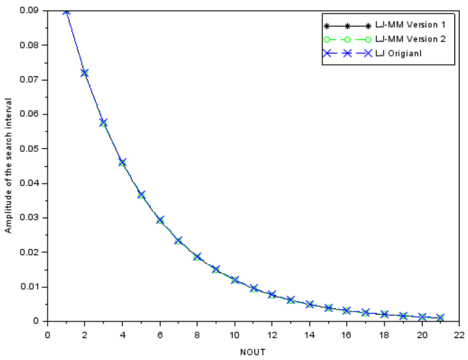
According to Jezòwski *et al.* (2005), the performance of the LJ-MM approach depends slightly on the initial solution candidates and parameter setting. This can be a critical point for the convergence of the solution, because in both cases comes up very fast there is an ideal solution, and the method can no longer find another great solution, unlike Original LJ.



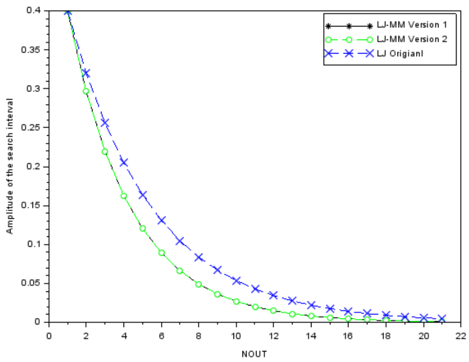
(a) Amplitude of the search interval for parameter α



(b) Amplitude of the search interval for parameter n

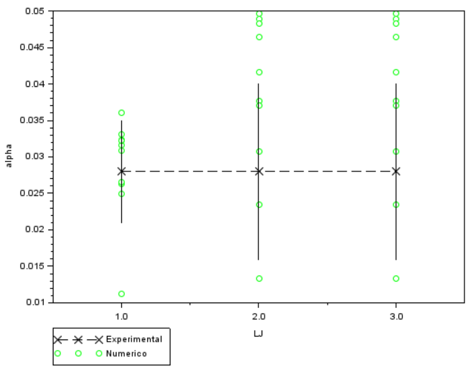


(c) Amplitude of the search interval for parameter θ_r

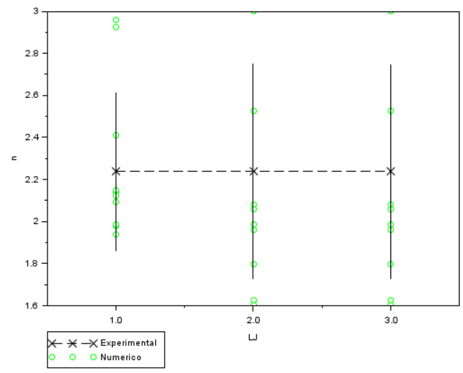


(d) Amplitude of the search interval for parameter θ_s

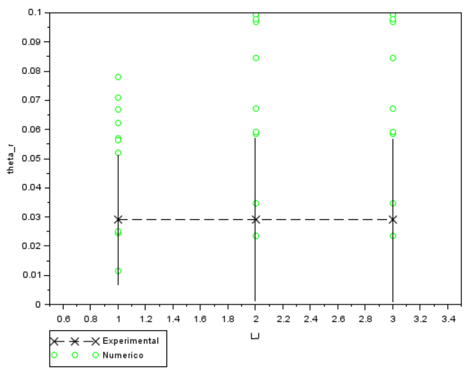
Figure 3. Analysis of the reduction of the search interval of the 10 runs.



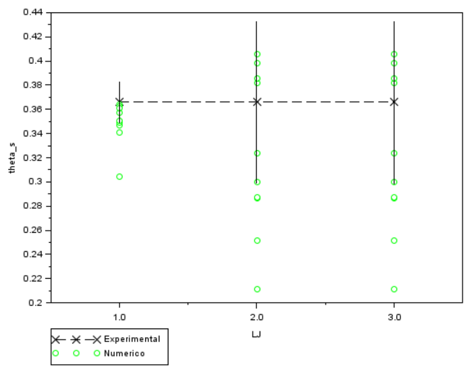
(a) Standard deviation for parameter α



(b) Standard deviation for parameter n



(c) Standard deviation for parameter θ_r

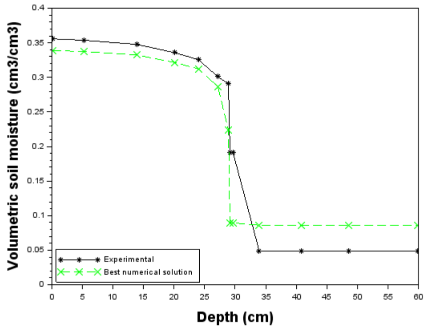


(d) Standard deviation for parameter θ_s

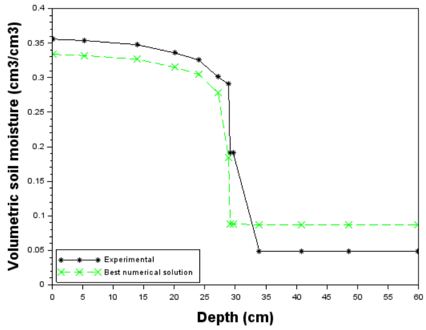
Figure 4. Analysis of the standard deviation of the 10 runs.

With a setting with $NOUT = 150$ and $NINT = 50$ the Original LJ yielded an excellent result.

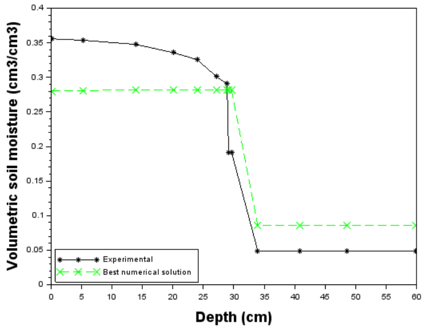
In the Figure 6 the data distributions obtained with the 10 rounds of each method are presented. We used the settings $NOUT = 10 \times NINT = 80$ to LJ original. To the LJ-MM Version 1 and Version 2 the parameters have been optimized



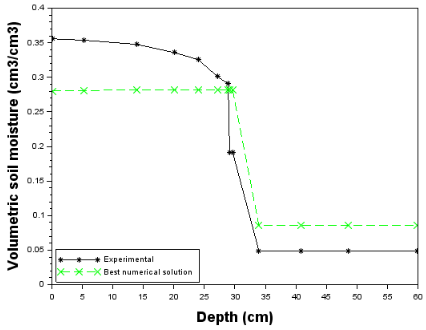
(a) LJ original: $NOUT = 10 \times NINT = 80$



(b) LJ original: $NOUT = 20 \times NINT = 50$

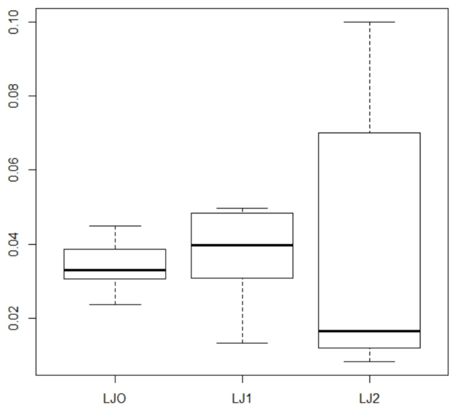


(c) LJ-MM Version 1: $NOUT = 20 \times NINT = 50$

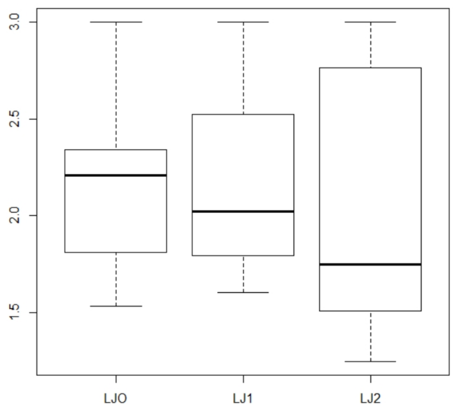


(d) LJ-MM Version 2: $NOUT = 20 \times NINT = 50$

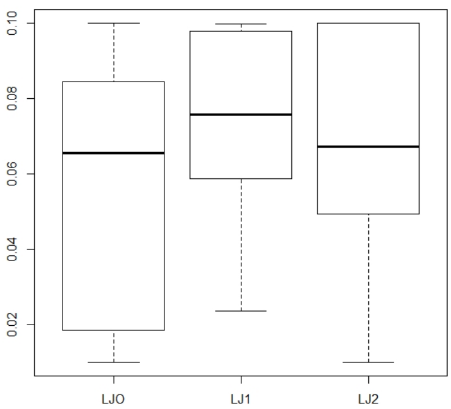
Figure 5. Volumetric soil moisture content evaluated using the parameters obtained with the LJ method.



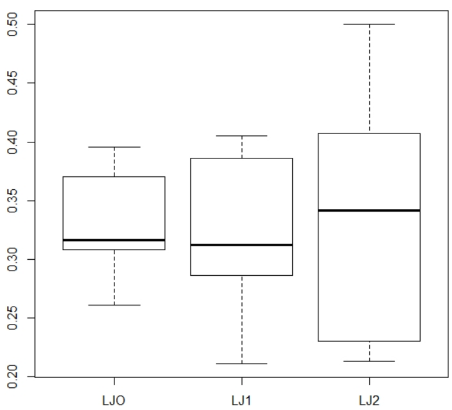
(a) Parâmeter α



(b) Parameter n



(c) Parameter θ_r



(d) Parameter θ_s

Figure 6. Boxplot to parameters α, n, θ_r and θ_s obtained with three versions of LJ Method.

with a new setting, $NOUT = 100 \times NINT = 50$. Better results were expected with this new configuration, however it is observed that even with a larger configuration, that is, with more random fetch, the LJ Original got better results.

4. CONCLUSIONS

After analyzing the results obtained with the three versions of the Luus-Jaakola method, original and LJ-MM version 1 and 2, it is found that the original LJ returned the best result. The original LJ is smoother in reducing the search interval, thus providing that the method does not get stuck on local solution candidates.

5. ACKNOWLEDGEMENTS

The authors acknowledge the financial support provided by FAPERJ, CNPq and CAPES (finance code 001), CNPq (processo 435238/2018-3 and 308363/2014-0).

6. REFERENCES

Celia, M.A., Bouloutas, E.T. and Zarba, R.L., 1990. "A general mass conservative numerical solution for the unsaturated flow equation". Vol. 26, No. 7, pp. 1483–1496.

de Vasconcellos, C.A.B. and Amorim, J.C.C., 2001. "Numerical simulation of water infiltration in homogeneous, non-saturated porous media (in portuguese)". XIV Simpósio Brasileiro de Recursos Hídricos, ABRH, Aracaju-SE.

Guterres, M.X., 2013. *Evaluation of the algorithms of Picard-Krylov and Newton-Krylov in the solution of the Richards equation (In Portuguese)*. Ph.D. thesis, IPRJ/UERJ, Nova Friburgo. Tese de doutorado.

Guterres, M.X., Vasconcellos, J.F.V., Silva Neto, A.J., Peralta, C.B.L. and Teixeira, L.G.M.F., 2017. "Approximation of a solution for the richards 2d equation by the finite volume method with the aid of the picard-krylov algorithms (in portuguese)". Vol. 31:2:89-108.

Jezòwski, J., Bochenek, R. and Ziomek, G., 2005. "Random search optimization approach for highly multi-modal non-linear problems". *Advances in Engineering Software*, Vol. 36, pp. 504–517.

Kroes, J.G., van Dam, J.C., Groenendijk, P., Hendriks, R.F.A. and Jacobs, C.M.J., 2017. "Swap version 4. theory description and user manual". Technical Report 1649 (02), KWR Watercycle Research Institute, Wageningen Environmental Research (Alterra), Alterra Repor, Wageningen.

Luus, R. and Jaakola, T.H.I., 1973. "Optimization by direct search and systematic reduction of the size of search region". *AIChE Journal*, Vol. 19, No. 4, pp. 760–766.

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

Silva Neto, A.J., Becceneri, J.C. and Campos Velho, H.F., 2016. *Computational Intelligence Applied to Inverse Problems in Radiative Transfer (In Portuguese)*. EdUERJ.

Silva Neto, A.J. and Moura Neto, F.D., 2005. *Inverse Problems: Fundamental Concepts and Applications (In Portuguese)*. Rio de Janeiro, RJ, Brasil.

Silva Neto, A.J. and White, R.E., 1994. "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*, Vol. 8-10, pp. 353–371.

Telles, W.B., 2014. *Prediction of the hydraulic behavior of a river based on the estimation of coefficients that control its flow. Case study: Bengalas River, Nova Friburgo-RJ (In Portuguese)*. Ph.D. thesis, IPRJ/UERJ, Nova Friburgo. Tese de Doutorado.

Temperini, M.O., 2018. *Inverse Modeling to Obtain Parameters for the Richards Equation (In Portuguese)*. Ph.D. thesis, PGEB/UFF, Niterói. Dissertação de Mestrado.

7. RESPONSIBILITY NOTICE

The authors are the only responsible for the printed material included in this paper.