

A free GUI application for solving the van Genuchten parameters using non-linear least-squares minimization and curve-fitting

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Abstract: The van Genuchten formulation for describing the water retention model of an unsaturated medium is among the most popular and commonly used. Proper estimation of its parameters is therefore very important. We present a graphic user interface software "vGS" that uses non-linear least-squares to solve these parameters.

Introduction

The van Genuchten water retention model is used to describe the physics of the soil in the forward hydrogeological modeling process (van Genuchten, 1980). In a saturated medium, the water flows through the soil at the speed defined by the saturated hydraulic conductivity K_s of the soil. In an unsaturated medium, the soil's pores are filled with a mixture of water and air, and the pressure head is negative (or the suction head is positive). When the pores are small, the effect of suction (capillarity) is high. In this scenario, the hydraulic conductivity K of the soil will be weaker than K_s and the ability for the soil to retain water will be high. The van Genuchten water retention model allows us to determine the hydraulic conductivity and the effective saturation (or water content) of an unsaturated soil as a function of suction head. In the field or in the laboratory, the water content and the pressure head can be determined using the instantaneous profile method during wetting and drying (Krisdani, 2009; Watson, 1966). The saturated hydraulic conductivity can be estimated using empirical or semi-empirical equations (Rosas et al., 2014) or through the use of advance hydrogeophysical techniques (Chou et al., 2014; Chou, 2015; Chou et al., 2016).

If the water content (or effective saturation) and the hydraulic conductivity of the soil are measured for a given suction head, the van Genuchten parameters can be determined. This can be done through numerical coding in Matlab, Excel spreadsheet, etc... In this paper, a graphic user interface software GUI called vGS, is developed to estimate the van Genuchten parameters using the non-linear least-squares method. It can also generate curves that fit over the field data points. Finally, this software is coded in Python and runs on Windows.

Theory

The van Genuchten water retention model is defined by equations 1 through 3.

$$Se = \begin{cases} \left[1 + \left|\alpha H_{P}\right|^{n}\right]^{-m} & H_{P} < 0 \\ 1 & H_{P} \ge 0 \end{cases}$$
 [1]

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$$k_r = Se^{l} \left[1 - (1 - Se^{-m})^m \right]^2$$
 [2]

$$K = K_{c}k_{r}$$
 [3]

There are 4 van Genuchten parameters $(\alpha, n, l, \text{ and } K_s)$. α (m⁻¹) is related to the inverse of suction, n and l are the curve shape parameters for the van Genuchten function, $m = 1 - m^1$, Se is the effective saturation, k_r is the relative hydraulic conductivity, K_s is the saturated hydraulic conductivity and H_P (m) is the pressure head. When the pressure head is positive, the soil is saturated and the pores are only filled with water.

The water content of the soil can be converted to the effective saturation by use of the following equation,

$$Se = \frac{\theta - \theta_r}{\theta_S - \theta_r} \tag{4}$$

where θ is the water content (water volume fraction), θ_S (m³m⁻³) is the total porosity, and θ_r (m³m⁻³) is the residual water volume fraction.

Method

In order to determine the van Genuchten parameters, equations 1 through 3 need to be solved. Due to the nonlinearity of the equations, a high-level interface to non-linear optimization is used to solve these equations (Newville et al., 2015). The root-mean-squared, RMS, is also calculated in order to determine the quality of the fit of the estimators to the data. The RMS is defined by the following equation,

$$RMS = \sqrt{\frac{1}{n} \sum_{i=1}^{n} \left(\frac{y_i - Y_i}{Y_i}\right)^2}$$
 [5]

where y_i represents the estimated value, Y_i represents the observed field value, and n is the number of data points.

Example

vGS can be obtained on the website www.cmcsjc.com. The file contains 2 demo dataset: Demo(Se-Hp).txt and Demo(K-Se-Hp).txt (Figure 1). If only the effective saturation and the suction head are known, equation 1 can be solved. The dataset Demo(Se-Hp).txt contains the effective saturation and the suction head that are calculated using the van Genuchten equations for parameters of a loamy sand (De Jong van Lier et al., 2009; Wösten et al., 2001). The dataset Demo(K-Se-Hp).txt is obtained the same way as the previous dataset where now the hydraulic Chou, T.K. (2016). A free GUI application for solving the van Genuchten parameters using non-linear least-squares minimization and curve-fitting, www.cmcsjc.com. January:1-5.



conductivity is also calculated. For each of these 2 datasets, vGS accurately determined the true van Genuchten parameters (Table 1). The RMS values are very low in both cases and the reconstructed curves fit also very well to the dataset (Figure 2 in the Appendix A).

Table 1. True (original) and determined van Genuchten parameters for the loamy sand using vGS.
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Parameters	Loamy Sand	Demo(Se-Hp).txt	Demo(K-Se-Hp).txt
α (m)	1.440	1.440	1.440
n	1.534	1.534	1.534
m	0.348	0.348	0.348
Ks (m/s)	1.785E-06	-	1.785E-06
1	-0.22	-	-0.215

Demo(Se-Hp) - No	ote		Demo(K-Se-Hp) - I	Notepad	_	
File Edit Format	View Help		File Edit Format	View Help		
0.010000000 0.017782794 0.031622777 0.056234133 0.100000000 0.177827941 0.316227766 0.562341325 1.000000000 1.778279410 3.162277660 5.623413252 10.000000000 17.782794100 31.622776600 56.23413252 10.00000000000000000000000000000000000	0.999479757 0.998743719 0.996972439 0.992738798 0.982781375 0.960209246 0.912916352 0.827379033 0.703215559 0.56215753 0.430860007 0.32280797 0.23929218 0.176560329 0.130017843 0.095665612 0.070365627	- III	0.010000000 0.017782794 0.031622777 0.056234133 0.100000000 0.177827941 0.316227766 0.562341325 1.000000000 1.778279410 3.162277660 5.623413252 10.000000000 17.782794100 31.622776600 56.23413252 10.00000000000000000000000000000000000	0.999479757 0.998743719 0.996972439 0.992738798 0.982781375 0.960209246 0.912916352 0.827379033 0.703215559 0.562157530 0.430860007 0.322807970 0.239292180 0.176560329 0.130017843 0.095665612 0.070365627	1.4337E-06 1.3172E-06 1.1675E-06 9.8070E-07 7.5895E-07 5.1750E-07 1.2644E-07 4.0825E-08 1.0241E-08 2.1825E-09 4.2711E-10 8.0358E-11 1.4863E-11 2.7292E-12 4.9964E-13 9.1358E-14	- H
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Figure 1. A look inside the demo data files (left: Demo(Se-Hp).txt and right: Demo(K-Se-Hp).txt).

Conclusion

A free van Genuchten parameters solver **vGS** is coded. Non-linear least-square method is used to solve the non-linear van Genuchten equation. Using synthetic data representing a loamy sand, vGS accurately estimated the original value. It is important to note that the accuracy of the result depends also on the quality of the dataset. In both examples, the data were free from any error. In field and lab measurements, data are prone to error such as instrument uncertainty and other technical difficulties encountered though the use of the instantaneous profile method. This GUI program is developed to facilitate users to quickly estimate the van Genuchten parameters and also as a learning tool.

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References

Chou, T.K., Chouteau, M.C. and Dubé, J.-S. (2014). Estimation of hydraulic conductivity for an heterogeneous unsaturated soil using electrical resistivity and level-set methods. COMSOL 2014 Conference in Boston.

Chou, T.K. (2015). Détermination de la conductivité hydraulique à saturation d'un sol non saturé par suivi d'infiltration à l'aide de la tomographie de résistivité électrique. École Polytechnique de Montréal. PhD Thesis.

Chou, T.K., Chouteau, M.C. and Dubé, J.-S. (2016). Estimation of saturated hydraulic conductivity with the aid of ERT. Vadose Zone Journal. *In review*.

De Jong van Lier, Q., Neto, D.D. and Metselaar, K. (2009). Modeling of transpiration reduction in van Genuchten-Mualem type soils. Water Resources Research. <u>45</u>:W02422.

Krisdani, H., Rahardjo, H. and Leong, E.-G. (2009). Use of instantaneous profile and statistical methods to determine permeability functions of unsaturated soils. Canadian Geotechnical Journal. <u>46</u>:869-874.

Newville, M., Stensitzki, T. and others (2015). Non-linear least-squares minimization and curve-fitting for Python. University of Chicago: Center for Advanced Radiation Sources.

van Genuchten, M.Th. (1980). A close-form equation for predicting the hydraulic conductivity of unsaturated soils. Soil Science Society of American Journal. <u>44</u>:892-898.

Watson, K.K. (1966). An instantaneous profile method for determining the hydraulic conductivity of unsaturated porous materials. Water Resources Research. $\underline{2}(4)$:709-715.

Wösten, J. H. M., Veerman, G. J., de Groot, W. J. M. and Stolte, J. (2001). Water retention and hydraulic conductivity characteristics of top and subsoils of the Netherlands: the staring-series. (In Dutch.) ALTERRA report no 153, Alterra, Wageningen.

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Appendix A

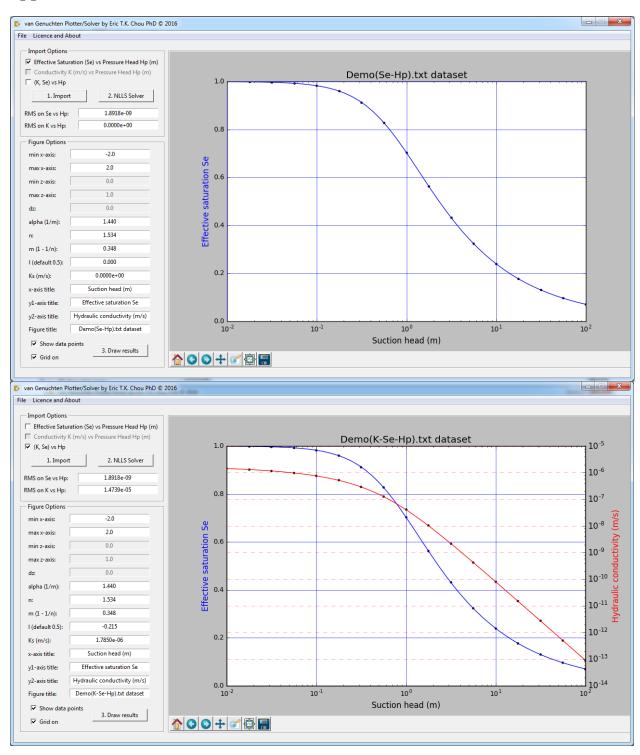


Figure 2. Top: Reconstructed water retention curve using the dataset Demo(Se-Hp).txt. Bottom: Reconstructed water retention curve (blue curve) and the hydraulic conductivity as function of suction head (red curve).

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