

Description of the program VGS to estimate soil hydraulic parameters

General

The FORTRAN code „VGS“ performs the fitting of the vanGenuchten/Mualem model (vanGenuchten, 1980) or of the fractal model after Soto et al. (2017) either to data of the water retention function (WRC) or simultaneously to water retention and soil hydraulic conductivity data (HCF). If parameters are fitted to water retention only, results are used to predict unsaturated soil hydraulic conductivity. The fitting method follows the Fibonacci algorithm (Vardavas, 1989, Leonardo da Pisa (Fibonacci), 1202).

Van Genuchten model

The model yields soil water content as function of soil water pressure head $\theta(h)$ und reads

$$\theta(h) = \theta_r + \frac{\theta_s - \theta_r}{(1 + (\alpha h)^n)^m} \quad (1)$$

It has 4 unknown parameters to be fitted, namely θ_r , θ_s , α , and n . To apply an analytical solution of unsaturated soil hydraulic conductivity based upon Mualem's theory, the parameter m is fixed to $m=1-1/n$. Then, hydraulic conductivity is given by

$$K(h) = K_s \frac{\left[1 - (\alpha h)^{n-1} (1 + (\alpha h)^n)^{-m}\right]^2}{(1 + (\alpha h)^n)^{m\tau}} \quad (2)$$

In this equation, the saturated hydraulic conductivity K_s and the tortuosity coefficient τ are additional parameters, which are fitted together with $\theta(h)$ simultaneously to given observations of unsaturated hydraulic conductivity. If the fitting is done to $\theta(h)$ only, tortuosity is assumed to be $\tau=0.5$ and an approximation to K_s must be given in the input stream. This provides a prediction of unsaturated soil hydraulic conductivity from the water retention characteristic.

Soto Fractal model

Recently, Soto et al. (2017) described a fractal-based model of soil hydraulic functions. Their water retention model reads

$$\theta(h) = \theta_r (1 + (h/h_0)^{-\lambda}) \quad \text{for } h > h_a \quad (3)$$

$$\text{and } \theta(h) = 1 \quad \text{for } 0 \leq h \leq h_a$$

From the derivation of Equ.(5) (see Soto et al., 2017) it can be seen that λ has a relation to the fractal dimension D , which is given by $\lambda = 3 - D$. The parameter h_a represents the observed or assumed bend of the WRC indicating the air entry value and is given by

$$h_a = h_o (S_r / (1 - S_r))^{-\lambda} \quad (4)$$

In this equation, S_r is given by $S_r = \theta_r / \theta_s$. Thus, the fitting parameters are θ_r , θ_s , λ , and h_o .

Soto et al.(2017) provided equations to calculate hydraulic conductivity K on the basis of the Burdine and Mualem theories. For the Mualem method, they obtained

$$K_r(S_e) = S_e^{\frac{19-5D}{6-2D}} \quad (5)$$

with
$$S_e = \frac{\theta - \theta_r}{\theta_s - \theta_r} \quad (6)$$

Parameter optimization

The error function used is the root mean square error, RMSE

$$RMSE = \sqrt{\frac{\sum_i^n (y_i - \hat{y}_i)^2}{n}}$$

A general problem of any search algorithm is not to be trapped in a local minimum of the error function but to find the global minimum. Often this is achieved by using several initial estimates of the unknown parameters. The program introduced here uses the Monte Carlo technique to find hopefully initial estimates in the vicinity of the global minimum. The resulting error function is named RMSE(1), given in cm³/cm³ water content. This step gets executed for water retention data only. Parameter fitting is then improved by an iterative scheme of a search algorithm based upon the Fibonacci method (Vardavas, 1989, Leonardo da Pisa, 1202) yielding the goodness coefficient RMSE(2). For simultaneous fitting, RMSE(3) indicates the error function of log₁₀(K) with units got from the input stream. Our experience has shown, that for the Soto fractal model, the problem of finding a suitable set of initial estimates is rather severe.

Implementation

The program is written in FORTRAN 95 and can be compiled under Ubuntu Linux using the GNU FORTRAN compiler (gfortran). It should run under FORTRAN 77 as well.

Data input

Control coefficients

model =1 means vanGenuchten model, model=2 means Soto fractal model

ksimul=0 means fit to water retention data only

ksimul=1 simultaneous fit to water retention and unsaturated hydraulic conductivity

Both of these terms are keyboard inputs.

conds In case of simultaneous fitting, the given input is regarded as an initial estimate, otherwise it is used for the prediction of hydraulic conductivity.

Input file for fitting the water retention function:

first line: soil number, number of data points, saturated hydraulic conductivity

(units will propagate to results), free format, space-separated

second line: up to 20 values of soil pressure head, positively taken, free format, space-separated

third line: corresponding water content data, cm³/cm³ or vol%, free format, space-separated

Input file for simultaneous fitting

first line	soil number, number of water retention data points, number of hydraulic conductivity data points, saturated hydraulic conductivity
second line	up to 20 values of soil pressure head, positively taken, free format, space-separated, valid for soil water retention
third line	corresponding water content data, cm ³ /cm ³ or vol%, free format, space-separated
4 th line	up to 20 values of soil pressure head, positively taken, free format, space-separated, valid for unsaturated soil hydraulic conductivity
5 th line	corresponding hydraulic conductivity data points, free format, space-separated, units must correspond to given conds (see above), E-format is permitted

Since the terms “model” and “ksimul” are requested to be entered on the keyboard at start of the program, these settings remain in effect for all following soils. Any change of “model” or “ksimul” requires a new start of the program.

In the present version of the program, the name of the input file can be chosen (up to 8 characters). The parameter output file is named with prefix ‘out’ followed by the input file name. The second output file is named ‘HyCond’ and if not renamed duly it gets overridden by subsequent runs.

Explanation of test examples

There are two input files given. “wrctest” is a data file to fit the water retention function (wrc) and “hctest” is intended to be used for simultaneous fitting. At run time, both of these files can be used either to fit the van Genuchten function or the Soto fractal model. With regard to the output files, I think that the abbreviations of the headlines are self-explaining. Please keep in mind that it may be necessary to rename the output files before starting a new run.

The given examples are no observations but are the straight-forward results of the vanGenuchten/Mualem equations with assumed arbitrary parameters. According to our experiences, the parameter values represent a sandy loam (1), a sand (2), and a clay loam (4). The assumed parameters have been

soil	th-r	th-s	alpha	vgn	tau	conds
1	0.15	0.42	0.02	1.6	0.5	30 cm/d
2	0.1	0.4	0.2	1.7	-1	300. cm/d
3	0.0	0.5	0.05	1.15	0	5.0

As shown by the output files, the van Genuchten version was able to recover the assumed parameters very closely, except for the tortuosity parameter, which is known to be very insensitive. In contrast, the Soto fractal model does not fit completely to the van Genuchten/Mualem functions. It is nevertheless a reliable approximation.

References

Leonardo da Pisa
Liber Abaci, Pisa 1202

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VARDAVAS, I.M. (1989): A Fibonacci search technique for model parameter selection. – Ecological Modeling 48, 65-81, Amsterdam