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Short Communication

Predicting soil water retention curves based on particle-size distribution using a Minitab macro

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Soil water retention curves are essential for solving water flow problems, but direct measurement usually is laborious, time-consuming and expensive. Thus indirect methods using more easily measured soil properties are frequently used. The model of Arya and Paris (1981) [Soil Sci. Soc. Am. J., 45: 1023-1030] has been used widely to predict water retention curves based on particle-size distribution and bulk density. A major difficulty in the application of this model is determining the empirical parameter describing soil particle shape. Despite numerous efforts for alternative calibration of this parameter, the original Arya-Paris model remains pervasive and relevant for varying textured soils. We developed an easy-to-use spreadsheet-like Minitab macro to automate the parameter estimation for use with the Arya-Paris model. This method was tested on prairie soils from North Dakota, USA. Results showed that parameter estimation for soil water retention curves was improved by allowing both soil particle shape and particle density parameters to vary. The best estimates of shape factors varied from 1.08 to 1.44 and those for particle density ranged from 1500 to 2650 kg/m^3. The macro facilitates the rapid characterization of soil water retention relations and is applicable to other soil types.

Key words: Soil bulk density, soil particle shape, soil particle density, soil particle-size distribution, soil water retention curve, total porosity, Arya-Paris model.

INTRODUCTION

The soil water retention curve describes the relationship between soil water content and matric potential, and is essential for the quantitative description of soil water and nutrient flow and uptake by plants (Campbell, 1985; Warrick, 2003). Soil water retention characteristics are useful also for deriving the unsaturated hydraulic conductivity function, which is essential for soil water modeling (van Genuchten, 1980). However, soil water retention characteristics usually exhibit great variability in the field, and experimental measurements require a large number of soil samples, which is laborious, time-consuming and expensive. Therefore, indirect methods using easily measured soil properties, such as particle-size distribution, bulk density and soil organic matter content (Vaz et al., 2005), are frequently used to estimate the water retention characteristics.

The physicoempirical model of Arya and Paris (1981) represents one such indirect method that has received wide attention due to its intuitive nature and practical implications for describing soil water movement. The model correlates soil particle-size distribution with pore size distribution and uses the capillarity relationship to link pore size to the matric potential of soil. The soil water content is described as the summation of pore volume up to a particular size class, similar to the work of Marshall (1958).

To reflect the complex shape and dimension of soil particles, an empirical scaling parameter was introduced in the Arya and Paris model. This scaling parameter and the correct estimation of it to represent varying soil types has been a focus of numerous subsequent studies on different soil types (Yang et al., 1994; Basile and D’Urso, 1997; Vaz et al., 2005; Rezaee et al., 2011).

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Instead of using a constant shape factor as in Arya and Paris (1981), the calibration has been formulated variably as linear and logistic models (Arya et al., 1999), as function of water content (Vaz et al., 2005) and matric potential (Basile and D'Urso, 1997), and as fractal models of particle-size distribution (Tyler and Wheatcraft, 1989; Xu, 2004). Nonetheless, the original model by Arya and Paris (1981) has been shown to give the best results describing the soil water retention charcteristics in some cases (e. g. Rezaee et al., 2011), and can adequately describe the spatial variation of soils of varying texture (Nasta et al., 2009).

There are circumstances in agronomy and crop science studies where a limited budget does not permit a complete sample analysis of major soil hydraulic properties, but an estimation of the soil water potential-water content relationship for water/solute transport equations is needed. In such a situation, a quick method of obtaining the needed parameters, preferably in a spreadsheet-like format, is essential. The objective of this paper is to describe the use of a Minitab (Version 13.31, State College, PA, USA) macro we developed for estimating the Arya-Paris model parameters based on measured particle-size distribution and bulk density data. Considering the wide accessibility and easy-to-use nature of the Minitab software (www.minitab.com), we believe the macro described here is of potential use for other situations as well.

MATERIALS AND METHODS

Soil samples were collected from pastures in a mixed-grass prairie in southcentral North Dakota, USA under two levels of season-long cattle grazing: extremely heavy grazing (with 80 percent current-year herbage removal by yearling beef cattle during a growing season), moderate grazing (50 percent current-year herbage utilization) and an ungrazed exclosure (see Patton et al. 2007, for detailed site characteristics). All samples were collected from silty upland range sites with each of them being a composite sample from three soil cores. In the exclosure, eight samples (0.15 m intervals for the first 0.91 m depth, and 0.3 m intervals from 0.91 to 1.52 m depth) were collected. In both the moderately grazed and the heavily grazed pasture, only two samples were collected (from 0-0.15 m depth interval and from 0.76–0.91 m depth interval) due to the cost of the laboratory measurements. Soil bulk density was measured in the field condition with undisturbed soils according to Blake and Hartge (1986a) and soil particle density was measured using the pycnometer method as described in Blake and Hartge (1986b). The remaining measurements were all made using disturbed soils according to standard methods as described below. Soil particle-size was analyzed using the pipette method (Gee and Bauder, 1986) with organic matter, carbonates and soluble salts removed. The soil water retention (characteristic) curve was measured according to Klute (1986), including ten levels of suction pressure (at 0.1, 0.2, 0.33, 0.5, 1, 2, 3, 5, 10, 15 bar) and with organic matter, carbonates and soluble salts not removed before laboratory analysis.

Software RETC (van Genuchten et al., 1991) was used to fit the soil water content (θ)-soil water potential (h) relationship curves according to van Genuchten (1980):

$$\theta = \theta_r + (\theta_s - \theta_r)(1 + |\gamma \cdot h|^n)^{-m} \tag{1}$$

where θ_r and θ_s (m^3/m^3) are residual and saturated water contents, respectively, γ, n and m are empirical shape parameters estimated from curve-fitting with constraint n=1/(1-m). For depth 0-0.15 m, estimated parameters are θ_r =0.15, θ_s =0.71, γ =11.7, m =0.267; for depth 0.76-0.91 m, estimated parameters are θ_r =0.001, θ_s =1.081, γ =37.3, m =0.143. We observed that θ_s at the wet end of the retention curves was over-estimated compared with typical values in literature (van Genuchten et al., 1991). To deal with this problem, we looked for ways that enabled us to find the total porosity of the soils that could be used to constrain the curve-fitting in RETC and to obtain reasonable estimates for θ_s. Total porosity (f) can be computed as

$$f = 1 - \frac{\rho_b}{\rho_p} \tag{2}$$

where ρ_b and ρ_p (kg/m^3) are bulk density and particle density, respectively. As bulk density was measured for our soil samples, we only need to find ρ_p in order to find f. As ρ_p for our samples was not measured initially, it was estimated according to Arya and Paris (1981) (later ρ_p was experimentally measured and compared against the model-based estimations).

Arya and Paris (1981) proposed a model linking soil particle-size distribution to soil water potential. First, the cumulative particle-size distribution curve is divided into n fractions representing different particle ranges. The model translates particle size into pore size by the following equation (assuming soil particles are spherical in shape):

$$r_i = R_i \sqrt{\frac{4en_i^{1-\lambda}}{6}}\ , \tag{3}$$

where r_i and R_i (m) are the pore radius and particle radius for the ith particle-size range; e is the void ratio defined as $e = (\rho_p - \rho_b)/\rho_b$; n_i is the number of particles in the ith particle-size range; λ is a soil particle shape factor (α as in the Arya-Paris model). Once the pore radii are found (using Equation 3), the corresponding soil matric potentials (m) can be found by the equation of capillarity:

Table 1. Soil texture, particle density, particle shape factor and total porosity for different soil samples as estimated by minimizing the difference between predictions from the model of Arya and Paris (1981) and the lab-measured soil water retention data. Lab-measured particle density was compared against the estimated particle density.

Site (grazing history)	Depth	USDA textural class†	Sand	Silt	Clay	Bulk density	Total porosity	ARD‡	Shape factor	Particle density (estimated)	Particle density (measured)	% difference§
	m		%	%	%	kg/m^3				kg/m^3	kg/m^3	
Moderate	0-0.15	C	25.9	32.4	41.7	830	0.336	0.07	1.08	1500	2520	40
	0.76-0.91	C	21.3	37.5	41.2	1284	0.506	0.05	1.24	2600	2720	4
Heavy	0-0.15	CL	32.0	33.3	34.7	950	0.527	0.08	1.44	1600	2600	38
	0.76-0.91	C	19.3	35.1	45.6	1252	0.528	0.06	1.21	2650	2680	1
Exclosure	0-0.15	CL	36.6	35.8	27.6	986	0.509	0.12	1.38	1600	2530	37
	0.15-0.30	CL	38.4	32.6	29.0	1330	0.470	0.09	1.29	2650	2670	1
	0.30-0.46	CL	39.3	32.5	28.2	1322	0.402	0.03	1.33	2200	2680	18
	0.46-0.61	CL	43.5	28.8	27.7	1365	0.456	0.06	1.35	2200	2680	18
	0.61-0.76	SCL	49.5	26.8	23.7	1738	0.344	0.17	1.44	2650	2690	1
	0.76-0.91	SCL	45.4	27.1	27.5	1454	0.451	0.07	1.36	2650	2690	1
	0.91-1.22	L	42.1	31.2	26.7	1530	0.423	0.14	1.44	2650	2690	1
	1.22-1.52	CL	40.9	32.0	27.1	1551	0.415	0.10	1.41	2650	2650	0

†Abbreviations for soil texture class: C- Clay; CL- Clay loam; L- Loam; SCL- Sandy clay loam.
‡ "ARD" refers to the average relative discrepancy between predicted and measured water retention data according to Equation 7 (part of
outputs of the Minitab macro).
§ "% difference" refers to the relative difference between measured and estimated soil particle densities.

$$h_i = \frac{2\sigma\cos\omega}{\rho_w\, g\, r_i}, \tag{4}$$

where σ (N/m) is the surface water tension at the air-water interface; ω is the contact angle (assumed to be $\omega = 0$); ρ_w is the density of water (= 998 kg/m^3 at 20 ºC); g (m/s^2) is the acceleration due to gravity and r_i (m) is the pore radius (same as in Equation 3). Volumetric water content for pores with largest size class corresponding to ith particle-size range (θ_i) is found by progressively summing the volumes of pores smaller than and up to this upper limit size class:

$$\theta_i = \rho_b \sum_{j=1}^{i} V_j, \qquad i = 1, 2, \ldots, n, \tag{5}$$

where ρ_b (kg/m^3) is soil bulk density and V_j (m^3/kg) is the pore volume corresponding to the jth size class per unit sample mass, which is computed as

$$V_j = \frac{W_j\, f}{\rho_p}, \tag{6}$$

with W_j representing solid mass per unit sample mass in the jth particle-size range, ρ_p the particle density (kg/m^3) and f the porosity as defined in Equation 2 (here the cumulative particle-size distribution curve is divided into n fractions). This model can predict water retention curves for a range of potentials much wider than the limits of the lab-measured data. However, some parameters, especially the soil particle shape factor λ and soil particle density ρ_p, may be different for different soils. The particle density for mineral soils is usually assumed to be ρ_p=

Figure 1. Soil water retention curves for the 0-0.15 m soil depth interval from moderately grazed pasture. Solid circles: predicted values from the Minitab macro; open circles: measured data in laboratory.

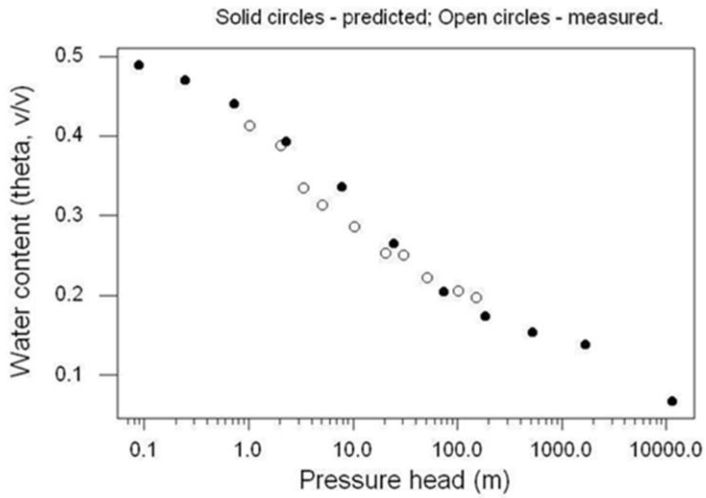
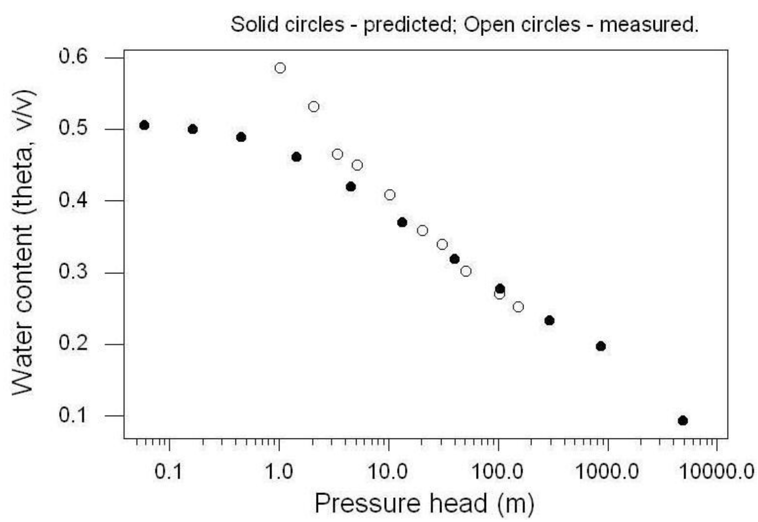


Figure 2. Same as in **Fig. 1**, but for the 0.76-0.91 m depth interval of soil.

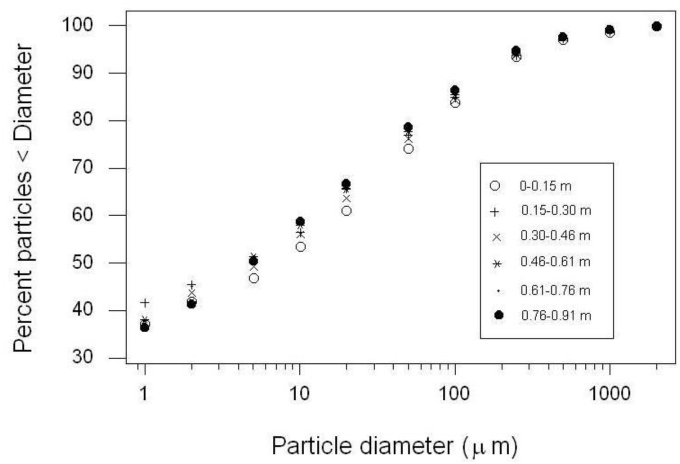


2650 kg/m^3 (Campbell, 1985). However, the average values of ρ_p could be as low as 1300 kg/m^3 when the soil contains a considerable amount of organic matter (Campbell, 1985). In our application, values of λ and ρ_p for our soils were allowed to change such that the differences between lab-measured and model-predicted water retention curve (using the Arya-Paris model) were minimized. This was measured by the average relative discrepancy as:

$$ARD = \frac{\sum_{i=1}^{k} |\theta_{mi} - \theta_{pi}|}{k \cdot \overline{\theta_m}}, \qquad (7)$$

where θ_{mi} and θ_{pi} (m^3/m^3) refer to measured and predicted soil water content for the ith data point, $\overline{\theta_m}$ is the average water content for the measured data points, and k is the total number of data points of one water retention curve. A Minitab macro was developed (see

Figure 3. Cumulative particle-size distribution curves for soil samples collected at six depth intervals from a moderately grazed pasture.



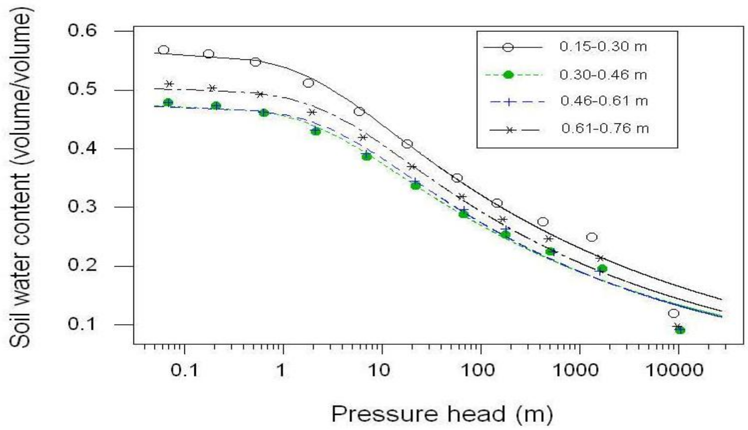
Supplementary 1) to automate the procedure of parameter estimation and create a visual comparison between predicted water retention data and measured ones. (The full dataset is included in Supplementary 2 for testing the macro.) Specifically, the following procedure was used to conduct a constrained curve-fitting for the lab-measured soil retention curves.

Each of the lab-measured soil particle-size distribution curves (see Supplementary 2 for original data) was divided into 11 particle-diameter ranges (1, 2, 5, 10, 20, 50, 100, 250, 500, 1000, and 2000 µm) and fitted to the model of Arya and Paris (1981). The averaged values of λ and ρ_p for our soil samples were estimated by a searching procedure that minimizes the relative discrepancy between the Arya-Paris model predictions and the lab-measured soil water retention curves as obtained in the previous step (through the Minitab macro). To enable an efficient computer search, the admissible values for λ and ρ_p were chosen as λ = 0.938-1.44 (divided into 51 equal steps), and ρ_p = 1250-2650 (kg/m^3,divided into 15 steps, see Supplementary 2 for the original data). These values were based on literature data (Arya and Dierolf, 1992; Arya and Paris, 1981; Campbell, 1985; Vaz et al., 2005). For each of the soil depth intervals, the Arya-Paris model was run multiple times, each with a different combination of a pair of admissible values of λ and ρ_p. The best value of ρ_p (i.e., one leading to the smallest relative discrepancy between lab-measured retention data and the Arya-Paris model predictions) was used to compute the total porosity using Equation 2. To accommodate for more diverse soil types and for a refined search for the best parameters values of the Arya-Paris model parameters (especially if one has a large sample of measurements), the Minitab macro described here allows for variable admissible parameter values other than the ones as used in this paper (see Supplementary 1 for detail).

RESULTS AND DISCUSSION

The best shape parameter λ for the twelve soil samples, as well as several other results, are shown in Table 1, and graphic outputs of the Minitab macro for two samples are shown in Figures 1-2. The application of the Arya-Paris model enabled a prediction of the θ-h relationship to a range of values much wider than those given from the lab-measured data (Figures 1-2). However, as shown in Figure 2, two wettest data points of the measured retention data deviate from the predicted data points. This occurred also in several other curves (data not shown). As we had suspected that these two wettest data points were due to the artifacts associated with soil disturbance (see above), we omitted them when using the RETC software to fit Equation 1 (Results are part of the input data for the Minitab macro; see Supplementary 2, columns “AO” through “AZ”). The estimated values for the soil particle shape factor λ (see Table 1) are comparable to the values given in Arya and Paris (1981), except the first sample of the moderate grazing pasture, which has a low value of 1.08. However, this low value is still within the range of λ values used by Arya and Dierolf

Figure 4. Predicted soil water retention characteristics using particle-size distribution (symbols) and the curves fitted to Equation 1 using RETC (lines). These are for the four soil depth intervals where no lab-measured retention data were available.



(1992) and Vaz et al. (2005). In the study of Vaz et al. (2005), λ = 1.38 provided a good estimation of the measured soil water retention characteristics for sandy soils, but a much lower value (λ = 0.977) better characterized the clay soils. Qualitatively, this is also seen in our results in that the best shape factor for soils with less clay content (such as those from the "Exclosure" site) tended to be higher than those with higher clay content (Table 1). However, three samples in our study reached highest admissible values (λ = 1.44), which may reflect the fact that the calibration shown in the current study allows both the shape factor and the particle density to vary, in order to find the best match between predictions from the Arya-Paris model and the model of van Genuchten (1980).

In our initial effort of model parameter estimation, we assumed a fixed ρ_p value 2650 kg/m^3(data not shown). However, this would lead to large differences between the model-predicted and the lab-measured water retention curves. Using a variable ρ_p, however, allowed a significant decrease in differences between the model-predicted and lab-measured retention curves. Considering the empirical nature of the Arya-Paris model, we think the use of variable ρ_p in our model-fitting exercise is acceptable. The very low ρ_p as estimated for the top soil layer, which is lower than the lowest measured value (2270 kg/m^3) for the surface layer of the same prairie soil (Volk, 2006), may be considered an apparent soil particle density, taking into consideration the fact that the top soil layer contains a large amount of organic matter. It is not surprising that for the top soil depth this apparent particle density is much lower than the density of mineral soil particles as measured in the lab (as shown in Table 1). The estimated ρ_p for depth intervals greater than 0.15 m are comparable, or slightly lower, than the literature data (Campbell, 1985; Volk, 2006), except the 0.3-0.46 m and 0.46-0.61 m depth intervals in the exclosure, for which the estimated ρ_p was 18 percent lower than the lab-measured value. Further study is needed to explain these differences, but we suspect that this might reflect the measured higher root activities in 0.25-0.75 m depth interval in the ungrazed exclosure than grazed pastures of the same study site (Volk, 2006).

Figures 3 and 4 showed the results of applying the Minitab macro to predict soil water retention curves for samples collected from a moderately grazed pasture. There are some differences in the particle-size distribution data for the six depth intervals of our soils (Figure 3). For example, the sample from the 0-0.15 m depth interval has a lower percentage of particles ranging from 5 to 100 μm, compared with the five other samples. Also, the sample from the 0.15-0.30 m depth interval has a higher percentage of particles with diameters less than or equal to 1 μm, compared with the remaining samples. However, the general similarity exists in the appearance of these six particle-size distribution curves. According to Arya and Paris (1981), the similarity in particle-size distribution suggests a similarity in water retention characteristic. As a result, we used measured particle-size data and bulk density data to estimate the water retention curves for the soil depth intervals where water retention curves were not measured in the laboratory (in order to limit the cost). This refers to the four soil depth intervals from 0.15 to 0.76 m (see Figure 3). We assumed that the same parameters for the sample of the

0.76-0.91 m depth interval (ρ_p = 2600 kg/m^3 and λ = 1.24) applies to those four depth intervals. The output data points were fitted to Equation 1 using RETC and compared against the output data from the Arya-Paris model (Figure 4).

Equations have been developed to consider the shape factor (λ) of the Arya-Paris model as a function of soil water potential (Basile and D'Urso, 1997) or soil water content (Vaz et al., 2005). Rezaee et al. (2011) compared a number of methods for optimal estimation of the shape factor. These attempts have led to improved accuracy in the predicted soil water retention curves. While it is interesting to investigate the similar relations for prairie soils as used in this study, the sample size of our current study is too small for a reasonable statistical analysis. Even though, our work demonstrates how to obtain the Arya-Paris model parameters with limited samples. This has practical implications in that this method is an alternative to the collection of hundreds of soil samples for detailed hydraulic property analysis. Meanwhile, as shown by Dong et al. (2010), the use of the soil water retention curves based on the Arya-Paris model not only improved accuracy of soil water prediction but also increased the sensitivity of soil water content to rain pulses at both the surface and sub-surface soil depths.

CONCLUSIONS AND RECOMMENDATION

A complete documentation of the detailed procedures of soil water retention curve analysis, along with the fully annotated computer code as shown in this paper, may be used for characterizing soil water parameters in similar and other related agricultural and environmental applications. The data, analysis and computer code from this study suggest research implications and potential applications for similar studies beyond the subject area:

1. The parameter estimation for soil water retention curves based on the Arya-Paris model can be improved by allowing both the soil particle shape parameter and particle density parameter to vary. This is relevant for most agricultural soils with high organic matter due to soil-microbial-plant interactions in the rhizosphere, but has not been emphasized in the literaure.
2. The spreadsheet-like Minitab macro developed in this paper is applicable for other soil types to facilitate a rapid estimation of soil water retention parameters. The following guidelines are recommended:

a. To run the macro, the measured data (cumulative soil particle-size distribution, soil bulk density, and soil water retention curves) must be copied into a Minitab worksheet (see Supplementary 1 and 2 for detailed instructions).

b. The user is assumed to provide customary admissible values for both the particle density (in column *X* of Supplementary 2; or column 24 in a minitab worksheet) and particle shape factor (in column *Y* of Supplementary 2; or column 25 in a minitab worksheet) at arbitrary lengths.

c. The current macro allows for 20 curves to be analyzed; if one has more curves, one can analyze them in batches of 20 curves. Each of the curves is to be processsed separately and the user is required to specify the appropriate data columns to use for processing each curve (again see the documentation of the macro as included in Supplementary 1).

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gmacro
arya

# The purpose of this MINITAB macro is to estimate soil water
# retention curves based on particle-size distribution
# and bulk density data according to L. M. Arya and
# J. F. Paris, 1981, SSSAJ 45: 1023-1030.

##### Revised version: Nov. 10, 2014
# Author:
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#
##### Major changes made in the revised version:
#
#     The limitation on admissible values of scaling factor
#     alpha(lambda in main text) and soil particle density (ro_p)
#     has been removed. So, more admissible values can be used
#     by expanding the list in columns X(ro_p) and Y(alpha) of the
#     supplementary file 'Dong-Suppl_2.xlsx'.
#     However, with a long list of admissible values, the computer
#     time needed to complete the search process will increase.
#####



##### Original version: Nov. 27, 2012
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#####

# This macro is used as supplementary material to the paper
# entitled "Predicting soil water retention curves based on
# particle-size distribution data using a MINITAB macro",
# by X. Dong and B. Patton, submitted to
# African Journal of Soil Science.


# Why MINITAB?
# Because the computing work required to complete this task
# is relatively small, I chose to use MINITAB macro to do it,
# instead of using a general purpose programming language.
# Besides, in MINITAB data storage and plotting is handy for
# quickly comparing the estimated soil water retention data
# against the measurements.


#################################################################
#  Read this section if you are not familiar with MINITAB.
#################################################################
# (1) MINIAB can be found at:
#     http://www.minitab.com/en-US/default.aspx
# (2) In this macro, all data is stored in one of the following
#     two ways: (a) as CONSTANTS, and (b) as COLUMNS (ARRAYS).
# (3) In MINITAB, constants can hold real/integer numbers having
#     default names k1, k2,.... Constants can have their nicknames.
#     For example, MINITAB command "name k1 'variable_1'" will
#     assign constant k1 a nickname "variable_1".
# (4) Arrays (here we only use 1-dimensional arrays) are stored in MINITAB
#     in different columns, designated as C1, C2,..., for column 1,
#     column 2, etc. Columns (arrays) can also have nicknames, but like
#     constants, it is much easier to use default names when indexing a
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#    variable in a macro.
# (5) A very useful programming feature is MINITAB's CK convention.


#    Assuming k1=2, either of the following two commands will print
#    the value of the second element of array C1 on the session widow:
#
#                "print C1(2)"
#
#                    or
#
#                "print C1(k1)"
#
#    Thus, MINITAB's "CK" convention can be useful for writing
#    a loop structure or a conditional structure by treating k1
#    as an index variable.
# (6) Finally, please note that Minitab is NOT case sensitive (thus,
#     "c1" is interpreted as the same as "C1").
#####################################################################



####################################################################
#                        Required user inputs (in Minitab worksheet)
####################################################################
# (1) The sample spreadsheet data file (Dong-Suppl_2.xlsx) must be
#    copied into a Minitab worksheet, with the 1st column of the
#    Excel file being copied into the first column of the Minitab
#    worksheet, and first row of the Excel file (labels)
#    in the header row of the Minitab worksheet.

# (2) Particle-size data are stored in c1-c21, where c1 is
#    for the particle diameter in micrometer and c2-c21 are for
#    accumulative percentages of different ranges of particle sizes.
#    I allocated the needed space to hold 20 samples of soil
#    particle-size distribution data. However, if you have more data,
#    you may analyze them in batches of 20 samples each.

# (3) Other measured data are stored in c23-c52. In particular,
#    c23: measured bulk density (kg m^{-3}) stored in rows 2-21,
#    where row 1 of c23 was deliberately left empty in order that
#    the row number of c23 and column number of c2-c21 index
#    the same soil samples (this simplifies the MINITAB macro).

# (4) c24 and c25: store possible values for particle density
#    (kg/m^3, ro_p) and shape factor (unitless, alpha).
#    Based on Arya and Paris (1981) and other related publications,
#    such as Vaz et al (2005), 15 possible values of
#    particle density (from 1250 to 2650 kg/m^3) and 51 possible
#    values of
#    alpha (from 0.938 to 1.440) are used in order for the macro to
#    find a best pair of values {ro_p, alpha} that minimizes the
#    difference between the measured and the estimated retention data.
#    However, other admissible values of different lengths can be used
#    as well (user should note that more admissible values
#    may lead to longer time for the Minitab macro to complete the
#    full search).
#
# (5) c41-c52: These columns are reserved for storing the parameters
#    of the model of Genuchten (1980) (see Eq. 1 of main text) as fitted
#    to measured soil water retention curves. This must be done using
#    other software such as
#    RETC (http://www.ars.usda.gov/News/docs.htm?docid=8952).
#    In each column, the fitted parameters must be placed in
#    this order: theta_r, theta_s, gamma, n, and m as defined in
#    van Genuchten's original paper.
###########################################################################



####################################################################
#            Instruction for processing individual samples
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###############################################################
#
# >>>  To process the 1st sample ("X 0-6", see Dong-Suppl_2.xlsx),
#        uncomment the following 6 commands AND comment out the
#        default values (for the 2nd sample as shown below)
# let k22=2
# let k33=27
# let k34=28
# let k44=41
# let k77=71
# let k78=72
#
# Definitions:
# k22: column number for accumulated percentage of particle-size data
# k33: column number for measured pressure head (m)
# k34: column number for measured theta corresponding to
#      measured pressure head (m).
# k44: column number for fitted parameters (th_r,th_s, gamma,
#      n, m) according to Genuchten (1980).
# k77: The destination column number for estimated pressure head (m).
# k78: The destination column number for estimated theta.

#     For the 1st sample "X 0-6":
#     C2 - the percentages of particle-size distribution;
#     C27 - measured pressure head data;
#     C28 - measured theta corresponding to measured
#         pressure head (m);
#     C41 - fitted parameters (th_r,th_s, gamma,
#         n, m) according to Genuchten (1980);
#     C71 - estimated pressure head (m);
#     C72 - estimated theta.
#
# >>>  If the 1st sample has been done, then the corresponding
#        commands must be commented out (see above). To process the 2nd
#        sample ("X 6-12", see Dong-Suppl_2.xlsx), make sure the
#        following 6 commands are active (here they are already
#        uncommented; that means this macro by default will process the
#        2nd sample, namely, sample "X 6-12", see Dong-Suppl_2.xlsx):

 let k22=3
 let k33=27
 let k34=29
 let k44=42
 let k77=73
 let k78=74

# >>>  To process other samples, the above 6 commands must be
#        edited accordingly (one should be able to do it after
#        inspecting the sample data file).

###############################################################



###############################################################
#                          OUTPUTS from the macro
###############################################################
# (1) The values of ro_p and alpha leading to the best fits
#      are printed out on the screen (MINITAB session window)
#      during the macro run.
# (2) The estimated retention curve is automatically compared
#     against the measured one graphically.
# (3) Estimated data of (water retention) are stored in c63-c86
#     (determined by constants k77 and k78)
# (4) Average relative discrepancies (ARD's) between measured and
#     and predicted water retention characteristics (c99),
#     as well as all the possible combinations of particle
#     density (c100) and alpha (c101) corresponding to the ARD's.
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#############################################################
#                         How to use it?
#############################################################
# (1) To use this macro, you first save this file in text format
#    in your computer (giving it a name 'arya.txt').
# (2) Save the sample Excel data file (or
#     equivalently, your own data file with same structure as this sample
#     file 'arya-input.xlsx') in your computer under the same folder.
# (3) Open the Excel data file 'arya-input.xlsx', select all the 86
#    columns and choose COPY; then Start MINITAB and under the DATA window
#    (in MINITAB it is called Worksheet) click on the upper-left cell
#    immediately under "C1", then choose PASTE within MINITAB (this will paste
#    the Excel data file into MINITAB). Make sure the data look right (the
#    column names are in the first row without a row number). Save this
#    MINITAB project file under the same folder, giving it a name (such as
#    "arya.mpj").
# (4) Now open this newly created MINITAB project file (by double-clicking it).
#    Click "session window" in MINITAB, which is the window to accept commands.
#    In this session window, if we don't see "MTB>" prompt followed by
#    a blinking curser, click "Editor/enable commands", so the prompt "MTB>"
#    is displayed.
# (5) Make sure the blinking curser is right after the "MTB>" prompt.
# (6) Assume the macro file has a name "arya.txt", we enter this command:
#
#                       %'arya.txt'
#
#     followed by Return. This will evoke the macro.
# (7) Depending on the number of the possible combinations of ro_p and alpha,
#     it may take minutes (e.g., 15 ro_p and 50 alpha values) to hours (if
#     hundreds admissible values are used) to complete the procedure.
# (8) When it is done, the macro will graph the data and print the optimal
#     pair of ro_p and alpha, along with the minimal relative error (ARD) in
#     the MINITAB session window. Detailed data are to be found in c99 to c101
#     within the current worksheet.
######################################################################


######################################################################
#                                    References
######################################################################
# 1. Arya, L. M., Paris, J. F., 1981. A physicoempirical model to predict
#    the soil moisture characteristic from particle-size distribution
#    and bulk density data. Soil Sci. Soc. Am. J. 45, 1023-1030.
#
# 2. van Genuchten, M. T. 1980. A closed-form equation for predicting
#    the hydraulic conductivity of unsaturated soils. Soil Sci. Soc.
#    Am. J. 44: 892–898.
#
# 3. Vaz, C. M. P., de Freitas Iossi, M., de Mendonca Naime, J., Macedo,
#    A., Reichert, J. M., Reinert, D. J., Cooper, M., 2005. Validation of
#    the Arya and Paris water retention model for Brazilian soils.
#    Soil Sci. Soc. Am. J. 69, 577-583.
######################################################################

let k198=count(c24)  # of admissible values of particle density
let k199=count(c25)  # of admissible values of scaling factor


set c99                        # column prepared for later use
0
end

let k55=0              # a flag
let k66=count(c99)+1
do k20=1:k198                  # particle density




 do k30=1:k199                 # alpha
   call arya1              # save ARD to c99, {ro_p, alpha} in c100-c101
 enddo
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```
enddo

Delete 1 c99-c101

let k90=min(c99)
let k3=count(c99)
do k2=1:k3
  if c99(k2)=k90
    goto 5
  endif
enddo
mlabel 5

name k1 'particle_density_kg/m3' k3 'best_alpha' k4 'average_error(ARD)'
let k1=c100(k2)
let k3=c101(k2)
let k4=c99(k2)
print k1 k3 k4
note
note
note The macro has run successfully!
note
note But you must check the results to make sure they are meaningful...

do k20=1:k198                    # k198 is number of possible ro_p values
  if c24(k20)=k1
    goto 10
  endif
enddo
mlabel 10

do k30=1:k199        # k199 is number of possible alpha values
  if c25(k30)=k3
    goto 15
  endif
enddo
mlabel 15

erase k1-k19 k21 k23-k29 k31-k32 k35-k43 k45-k76
erase k79-k90
erase c87-c134


# call arya1 but with known ro_p and alpha

let k55=1
call arya1               # graphing data

erase k1-k90
erase c87-c134

endmacro




gmacro
arya1

#  estimating the best ro_p and alpha
let k1=(c24(k20)-c23(k22))/c23(k22)       #e=(ro_p-ro_b)/ro_b
let c126(1)=ck22(1)
do k2=2:11
  let k3=k2-1
  let c126(k2)=ck22(k2)-ck22(k3)



enddo

let c126=c126/100                # W_i, will be used later
let c127=c126/c24(k20)*k1
let k4=1/c23(k22)                # V_b
let c127=c127/k4                 # V_vi/V_b
```

```
let k5=c127(1)
do k2=2:11
  let c127(k2)=c127(k2)+k5      # theta_vi
  let k5=c127(k2)
enddo

let c128(1)=c127(1)/2
do k2=2:11                                        # theta_Vi^*
  let k3=k2-1
let c128(k2)=(c127(k2)+c127(k3))/2
enddo

let c129(1)=c1(1)/2                # mean particle diameter in um
do k2=2:11
  let k3=k2-1
  let c129(k2)=(c1(k2)-c1(k3))/2+c1(k3)
enddo

let c129=c129/2*0.000001       # particle radius in m
let c130=3/4*c126/(3.14159*c129**3*c24(k20))      # n_i
let c131=4*k1*c130**(1-c25(k30))/6       #scratch variable for r_i
let c131=abso(c131)
let c131=c129*sqrt(c131)                  # r_i in m

let k6=0.0728                              # sigma in N/m
let k7=998                                 # ro of water at 20C in kg/m3
let k8=9.8                     # g in m/s^2
let c132=2*k6/(k7*k8*c131)     # psi_i in m

Sort c132 c128 c132 c128;
  By c132.

if k55=0
  call arya2                   # prepare the list of possible ro_p and alpha
else
  call graphi                  # given ro_p and alpha, compare with measurement.
endif

endmacro



gmacro
arya2

let c133=ck44(1)+(ck44(2)-ck44(1))*(1+(ck44(3)*c132)**ck44(4))**(-ck44(5))
let k9=mean(c133)
let c134=c133-c128
let c134=abs(c134)
let k10=mean(c134)
let k10=k10/k9                 # ARD


let c99(k66)=k10      # store ARD before leaving this sub
let c100(k66)=c24(k20)         # store ro_p before leaving this sub
let c101(k66)=c25(k30)         # store alpha before leaving this sub
let k66=k66+1
endmacro



gmacro
graphi

copy c132 ck77
copy c128 ck78

Plot C128*C132 Ck34*Ck33;
  Symbol;
    Type 6 0;
```

```
    Color 1;
    Size 1.0;
  Symbol;
    Type 0 1;
    Color 1;
    Size 1.0;
  LogScale 1;
  Overlay;
  ScFrame;
  ScAnnotation;
  Axis 1;
    Label "Pressure head (m)";
  Axis 2;
    Label "Water content (theta, v/v)";
  Tick 1;
    NMinor 9;
  Tick 2;
  Footnote "Solid circles - predicted; Open circles - measured.".
endmacro
```

Dong_Suppl_2

COLUMNS A-L

DIAMETER(UM)	X 0-6	X 6-12	X 12-18	X 18-24	X 24-30	X 30-36	X 36-48	X 48-60	M 0-6	M 6-12	M 12-18
1	25.7	26.5	24.7	23.4	19.3	23.9	23.3	21.6	37.1	41.6	37.5
2	27.6	29	28.2	27.7	23.7	27.5	26.7	27.1	41.7	45.4	43.7
5	32.9	32.3	33.4	34	29	32.7	32.9	30.2	46.7	50.8	49.3

10	38.4	37.2	38.6	38.6	33.4	38.9	39.5	37.6	53.4	56.5	56
20	45.8	44.9	44.1	45.6	40.8	44.7	46.7	46	61.1	65.7	63.6
50	63.4	61.6	60.7	56.5	50.5	54.6	57.9	59.1	74.1	76.9	76.2
100	74.9	73.3	71.3	66.8	59.5	63.7	68.2	69.9	83.9	85	84.5
250	86.3	84.8	84.5	81.6	75	78.8	83.1	83.3	93.6	94	94
500	93.3	92.3	92.4	90.6	86.4	89.7	91.9	91.8	97.1	97.5	97.8
1000	96.7	96.7	97	95.9	94.2	96.1	96.8	96.6	98.7	99.1	99.4
2000	100	100	100	100	100	100	100	100	100	100	100

COLUMNS M-W

M 18-24	M 24-30	M 30-36	H 0-6	H 6-12	H 12-18	H 18-24	H 24-30	H 30-36		BULK DENSITY
37.9	37.8	36.2	30.4	36.3	36	38.6	38.2	39.6		*
41.7	45	41.2	34.7	38.3	41	43.3	43.1	45.6		986
51.3	51	50.4	39.8	45.5	48	50.9	52.4	52.5		1330
58	58.1	58.7	46.3	51.6	54.2	57.6	59.7	59.4		1332
65.5	66.1	66.7	54.7	58.6	62.1	64.1	68.2	68.9		1365
77.7	77.9	78.7	68	70.7	74	77.3	79.1	80.7		1561
85.5	85.6	86.5	75.5	78.4	81.8	84.6	86.3	87.6		1454
94.4	94.4	94.8	86.7	89	91.8	93.5	94	94.7		1507
97.9	97.6	97.8	93.2	94.7	96.4	97.3	97.3	97.7		1551
99.4	98.9	99.2	97	97.4	98.7	99.2	99.1	99.3		830
100	100	100	100	100	100	100	100	100		1111
										1350
										1350
										1264
										1278
										976
										965
										1173

COLUMNS X-AF

PARTICLE DENSITY	ALPHA_1		HEAD(M)	TH-X06	TH-X612	TH-X1218	TH-X1824	TH-X2430

1250	0.938	1.02	0.38553	0.41323	0.40797	0.37701	0.51445
1350	0.948	2.04	0.36374	0.38876	0.36699	0.36336	0.46509
1500	0.958	3.36	0.29915	0.33543	0.31437	0.32514	0.39870
1600	0.97	5.1	0.27431	0.31415	0.29375	0.29429	0.36759
1700	0.98	10.19	0.26218	0.28582	0.26929	0.27027	0.31944
1800	0.99	20.38	0.24788	0.25297	0.23413	0.24720	0.28660
1900	1	30.57	0.23832	0.25017	0.22474	0.22482	0.26470
2000	1.01	50.95	0.21791	0.22198	0.20504	0.20393	0.23915
2100	1.02	101.9	0.20667	0.20575	0.18191	0.17199	0.19987
2200	1.03	152.85	0.19799	0.19764	0.17080	0.15766	0.18944
2300	1.04						
2400	1.05						
2500	1.06						
2600	1.07						
2650	1.08						
	1.09						
	1.1						
	1.11						
	1.12						
	1.13						
	1.14						
	1.15						
	1.16						
	1.17						
	1.18						
	1.19						
	1.2						
	1.21						
	1.22						
	1.23						

1.24
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1.36
1.37
1.38
1.39
1.4
1.41
1.42
1.43
1.44

Columns AG-AO

th-X3036	th-X3648	th-X4860	th-m06	th-m3036	th-h06	th-h3036	param-X06
0.491888	0.51515	0.48360	0.3765	0.5868	0.41401	0.62913	0.001
0.441725	0.45915	0.46747	0.3387	0.5322	0.39292	0.54187	0.543
0.373387	0.40958	0.40404	0.2918	0.4656	0.32576	0.48477	108.1
0.338491	0.38923	0.38232	0.2723	0.4499	0.32433	0.45535	1.104
0.307812	0.33538	0.34262	0.2518	0.4083	0.29479	0.41404	0.094
0.279895	0.28167	0.30167	0.2342	0.3589	0.27579	0.36834	

0.257358	0.26377	0.26445	0.2223	0.3394	0.26914	0.33604
0.226969	0.23394	0.22862	0.2099	0.3021	0.25023	0.29635
0.197162	0.21604	0.20411	0.1998	0.2703	0.24007	0.27006
0.17826	0.19997	0.18286	0.1827	0.2526	0.23883	0.248647

COLUMNS AP-AV

PARAM-X612	PARAM-X1218	PARAM-X1824	PARAM-X2430	PARAM-X3036	PARAM-X3648	PARAM-X4860
0.001	0.021	0.001	0.001	0.001	0.17	0.108
0.788	0.387	0.359	0.544	0.424	0.448	0.427
127.7	0.776	0.289	1.237	0.365	0.181	0.131
1.142	1.187	1.212	1.201	1.21	1.644	1.479
0.124	0.158	0.175	0.167	0.174	0.392	0.324

COLUMNS AW-AZ

PARAM_M06	PARAM-M3036	PARAM_H06	PARAM-H3036
0.0684	0.1508	0.001	0.129
0.4583	0.4984	0.475	0.527
9.24	0.16	16.78	0.202
1.1644	1.3838	1.091	1.349
0.1412	0.2774	0.083	0.259

COLUMNS BK-BM

HEAD-M06	TH-STAR-M06	HEAD-M3036

Columns BN-BU							
th-star-m3036	head-h06	th-star-h06	head-h3036	th-star-h3036	head-x06	th-star-x06	head-x612
Columns BV-CB							
th-star-x612	head-x1218	th-star-x1218	head-x1824	th-star-x1824	head-x2430	th-star-x2430	
Columns CC-CH							
head-x3036	th-star-x3036	head-x3648	th-star-x3648	head-x4860	th-star-x4860		