Estimating Parameters of Van Genuchten Model for Soil Water Retention Curve by Intelligent Algorithms

Abstract: An improved particle swarm optimization (IPSO) was proposed and the intelligent algorithms such as IPSO, genetic algorithm (GA), and simulated annealing algorithm (SA) were introduced to determine parameters of Van Genuchten (VG) model for soil water retention curve (SWRC) of four typical agricultural soil textures (clay, clay loam, silt loam and sand loam) in China. For comparison, the SWRC in term of VG model was also fitted by a computer program RETC and pedotransfer function Rosetta, respectively. For four soil textures, the value of determination coefficient (R^2) and root mean square error ($RMSE$) in the estimation of VG equation parameters by IPSO are the highest and lowest in the above three intelligent algorithms, respectively. The simulated values of water content by IPSO are much closed to the measured values ($R^2 = 0.990$). It was found that the Rosetta is unable to estimate the SWRC adequately and the highest $RMSE$ value is up to $1.096E-01cm^3cm^{-3}$. The predicted values of moisture content by Rosetta are far away from the measured values ($R^2 = 0.585$). The RETC provided good simulation results of water content ($R^2 = 0.974$). However, the soil residual water content (θ_r), of VG equation can not be obtained. It was concluded that the IPSO presented here is more reasonable and reliable to estimate the SWRC in term of VG model than the method of GA, SA, RETC and Rosetta.

Keywords: Soil water retention curve, Van Genuchten model, particle swarm optimization, genetic algorithm, simulated annealing algorithm, RETC, Rosetta.

1 Introduction

The soil water retention curve (SWRC), which is defined the relationship between soil water content and hydraulic potential, is an important physical property of soil material [1]. SWRC is indispensable when studying water flow processes and modelling water and solute movement through an unsaturated soil or when calculating the water availability for plants [2]. Empirical formulas are widely used to describe SWRC, where Van Genuchten (VG) equation is almost appropriate to all the soil textures [3]. However, four independent parameters need to be determined in VG equation, and the parameter fitting involves in the solution of nonlinear problems. Commonly-used least square method not only highly depends on the initial value of parameter, but also generates phenomena of algorithm termination and negative value.

Many researchers have been intended to solve these problems, which are mainly divided into the following 4 types.

(1) The optimization algorithms such as the nonlinear simplex method, Picard iterative approach, simplex evolutionary method and nonlinear damping least square were used to fit parameters of VG model [4, 5].

(2) The computer program, RETC [3], Data Processing System (DSP) and nonlinear function toolbox of MATLAB [6] were applied to estimate the VG equation parameters. However, the above approaches (1) and (2) strongly rely on the initial values of parameters. It is the same as the least square method.

(4) The VG equation parameters are indirectly estimated from basic soil properties such as sand, silt and caly fractions, bulk density, or water content at $-33kPa$ (corresponding to field capacity) and $-1500kPa$ (corresponding to permanent wilting point) using pedotransfer functions (PTFs) [9]. Bouma [10] introduced the term pedotransfer functions (PTFs), which was described as the predictive functions of certain soil properties from other easily, routinely, or cheaply measured properties. Rosetta is a pedotransfer function to estimate the parameters of VG model from surrogate soil

data such as soil texture data and bulk density [11]. Nevertheless, the errors between measured values of SWRC and predicted values determined from PTFs are larger than those of direct computation.

Therefore, a global optimization algorithm is urgently required to estimate parameters of VG model with a high accuracy. The new algorithm is hopefully independent on the initial values of parameters and the soil-column experiment is not required. Recently, the application of intelligent algorithm, such as generic algorithm (GA), particle swarm optimization (PSO) and simulated annealing algorithm (SA), has been introduced in hydrological sciences. However, no attempt on applying the intelligent algorithm to determine the SWCC was cited in the literature [12, 13]. Thus, the objective of this study was:

(1) Improve the method of particle swarm optimization (IPSO) to avoid falling into local optimal solution and appearing the premature phenomenon;

(2) Compare the performance of three intelligent algorithms, i.e. IPSO, GA and SA, on estimating the VG equation parameters for SWRC;

(3) Compare the simulated results of IPSO with those of RETC and Rosetta.

2 Van Genuchten Model

The VG equation was proposed by van Genuchten in 1980 [14] with the expression as below:

$$\theta = \theta_r + \frac{\theta_s - \theta_r}{[1 + |\alpha h|^n]^m} \tag{1}$$

where, θ is the soil water content ($cm^3 \cdot cm^{-3}$), θ_r is the soil residual water content ($cm^3 \cdot cm^{-3}$), θ_s is the soil saturated water content ($cm^3 \cdot cm^{-3}$), h is soil water potential (kPa), α is a scale parameter inversely proportional to mean pore diameter (cm^{-1}), n and m are the shape parameters of soil water characteristic, $m = 1 - 1/n$, $0 < m < 1$. Under the conditions of available measured data of the soil water content and water potential, the parameters of VG model can be estimated by the least square method, i.e.,

$$\min f = \sum_{i=1}^{N} (\theta_i - \theta(h_i, X))^2 \tag{2}$$

where, θ_i is the i-th measured soil water content ($cm^3 \cdot cm^{-3}$); h_i is the i-th measured soil water potential (kPa) corresponding to θ_i; $\theta(h_i, X)$ is the soil water content ($cm^3 \cdot cm^{-3}$) calculated by Eq.(1); $X(\theta_r, \theta_s, a, n)$ is the parameter vector to be optimized; N is the number of measured data.

It is required to quantify the amount by which an estimated value differs from the measured value of the quantity being estimated. Such quantification describes how well the estimator describes the measured values. In this research, such differences between estimated values and the measured values are quantified using the following performance criterion:

(1) root mean square error ($RMSE$)

$$RMSE = \sqrt{\frac{1}{n}(\sum_{i=1}^{N} P_i - M_i)^2} \tag{3}$$

(2) determination coefficient (R^2)

$$R^2 = 1 - \frac{\sum_{i=1}^{N} (M_i - P_i)^2}{\sum_{i=1}^{N} (M_i - \overline{M})^2} \tag{4}$$

where, P_i and M_i are the predicted and measured values of the i-th measured data, respectively; $\overline{M}$ is the mean of measured values.

3 Principle of numerical methods

3.1 Genetic algorithm

GA is a randomly searching algorithm based on biospheric natural selection and population genetic mechanism. According to the gradient or higher-order statistics of a single metric function (evaluation function), a traditional optimization algorithm is used to generate a deterministic sequence of test solution. However, GA does not rely on the gradient information. It searches the optimal solution by stimulating the natural process of evolution. GA uses a coding technology with the effects on digital strings (chromosome) to simulate the evolution process of population. Through organized random exchange of information, the digital strings with better adaptability are reconstructed by GA to generate new populations. In order to eliminate the disadvantages of the standard genetic algorithm, i.e., premature convergence, a large computational complexity and poor solution accuracy, the real-coded genetic algorithm integrated with Levenberg-Marquardt method [15, 16] was used to determine parameters of VG model in this research.

3.2 Simulated annealing algorithm

SA was proposed by Metropolis in 1953, and successfully applied in combinatorial optimization by Kirkpatrick et al. in 1983 [17]. The thermodynamic process of physical annealing is stimulated in SA, and the solution and objective function are corresponding to particle state and its energy respectively. For a given initial temperature, the temperature descends according to the attenuation function, and the globally optimal solution of objective function is randomly searched by Metropolis rule in the solution space. The standard SA [17] was employed to estimate VG eqaution parameters in this study.

3.3 Improved particle swarm optimization

PSO was jointly presented by a U.S. social psychologist James Kennedy and an electrical engineer Russell Eberhart in 1995 [18]. It was enlightened by the simulation results of birds behavior and the biological behavior model of Heppner and Grenander [19]. The basic PSO [17] is easy to fall into the local optimal solution and appear the premature phenomenon. To improve the basic PSO, an IPSO was proposed in this research. The new algorithm is a coupling of the constriction factor particle swarm optimization (CFPSO) of Clerk and Kennedy [20] and the PSO of Filedsend [21]. Although the convergence rate of CFPSO is fast, the diversity of species loses quickly and the premature convergence happens easily during the solution process. On the other hand, the species diversity of Filedsend PSO is good with computing procedure, but its global convergence rate is slow. Therefore, the improved PSO is proposed to inherit the advantages of the former two PSO models in order to overcome their shortcomings. Its basic principles of the IPSO are shown as follows.

It is assumed that a group is composed of M particles in the D-dimensional search space with a certain flight speed. x_i and v_i are the position and velocity vector of i-th particle respectively, i.e. $x_i = (x_{i1}, x_{i2}, \cdots, x_{id})$, $v_i = (v_{i1}, v_{i2}, \cdots, v_{id})$. $p_i = (p_{i1}, p_{i2}, \cdots, p_{id})$ is the optimal position for a single particle and $p_g = (p_{g1}, p_{g2}, \cdots, p_{gd})$ is the optimal position for all particles. In the iterative process, the velocity and position of particles are updated according to the following equation.

$$\begin{aligned} v_{id}^{t+1} = K(v_{id}^{t} + c_1 r_1 (p_{id}^{t} - x_{id}^{t}) \\ + c_2 r_2 (p_{gd}^{t} - x_{id}^{t}) + (p_{gd}^{t} - p_{id}^{t})) \end{aligned} \tag{5}$$

$$x_{id}^{t+1} = x_{id}^{t} + v_{id}^{t+1} \tag{6}$$

where, $i = 1, 2, \cdots, M$ and $d = 1, 2, \cdots, D$. t is the iteration number, r_1 and r_2 are random numbers distributed uniformly in [0,1], c_1 and c_2 are learning factors, K is the contraction factor ($K = \frac{2}{|2-\varphi+\sqrt{\varphi^2-4\varphi}|}, \varphi = c_1 + c_2, \varphi > 4$), $v_{id} \in [-v_{max}, v_{max}]$ and v_{max} is the maximum speed.

4 Materials and methods

4.1 Soil data

The soil properties of four agricultural soil samples were adopted for the analysis, which were cited from China Soil Scientific Database. The basic physical properties of soil samples are shown in Table 1. The soil moisture content was determined by the disturbed core samples on silt bath at pressure of 0, 1, 3 and 10kPa, kaolinite bath at pressure of 20 and 33kPa, and by the disturbed samples in high pressure pan at pressure of 250 and 1500kPa. Fig 1 displayed the SWRC of the four textures. It was found that the retention behavior of the textural classes is different from each other distinctly [22].

Table 1 Physical properties of four agricultural soil samples

Soil texture	Particle composition %			Bulk density
	Sand	Silt	Clay	
	2-0.05mm	0.05-0.002mm	$<0.002mm$	$/gcm^{-3}$
Clay	15.0	76.0	9.0	0.99
Clay loam	42.0	29.0	29.0	1.49
Silt loam	11.0	12.0	77.0	1.10
Sand loam	57.0	12.0	31.0	1.27

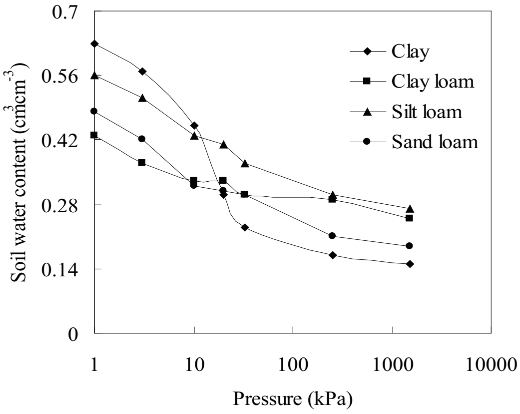

Fig. 1 Soil water retention curves for the four textures [21]

4.2 Parameters determination of numeric methods

The parameter setting of intelligent algorithm is a key factor that impacts the solution accuracy. According to the existing research results [23–26] and self-testing, the parameters of three intelligent algorithms were determined and was shown in Table 2. Rosetta offers five hierarchical sequences of input data: (1) soil textural class; (2) sand, silt and clay percentages; (3) sand, silt and clay percentages and bulk density; (4) sand, silt and clay percentages, bulk density and a water retention point at 33 kPa; (5) sand, silt and clay percentages, bulk density and water retention points at 33 and 1500 kPa. It was demonstrated that the comparison of observed and estimated SWRC showed an increase in the regression

Table 2 Parameter setting of the three intelligent algorithms

Intelligent algorithms	IPSO	GA	SA
Parameter setting	Population size=100	Population size=100	Boltzmann Contant=0.95
	Neighboring population size =2	Crossover rate =0.85	Maximum inner loop=100
	Maximum speed=2	Mutational rate=0.01	Cooling coefficient=0.9
	Learning factor c_1=2.05	Crossover=Uniform crossover	Initial temperature=999
	Learning factor c_2=2.05	Selection=Roulette wheel selection	Energy transformation model=Single-step transformation

coefficient R^2 value with an increase input predictors [27–30]. Therefore, the hierarchical level of item (5) of input data was used for this study.

5 Results and discussion

5.1 Performance of intelligent algorithm for estimating parameters of VG model

Although the initial value of parameter of VG model is not required for the intelligent algorithms, it would be very helpful to shorten the workload and calculation time if the possible range value of each parameter is given. Therefore, the range of the parameters was given for intelligent algorithms and it was determined according to the literatures [31, 32], where α was set as $0-1cm^{-1}$, θ_s was set as: $0.5-0.6cm^3cm^{-3}$ (clay), $0.4-0.5cm^3cm^{-3}$ (loam), and $0.3-0.4cm^3cm^{-3}$ (sand), θ_r was set as $0-0.2$ and n was between 1 and 10. Without loss generality, the possible value of VG equation parameters was chosen in the range of $\alpha \in [0,1]$, $\theta_s \in [0.3,0.6]$, $\theta_r \in [0,0.2]$, $n \in [1,10]$. The maximum iteration number of each algorithm was set to be 200. Each intelligent algorithm was run for 20 times and the solution of VG model corresponding to the lowest *RMSE* was listed in Table 3.

The R^2 values in the estimation of VG equation parameters are equal or greater than 0.960 by the three intelligent algorithms, see Table 3. The magnitude of *RMSE* varies from 0.00618 to 0.03596 cm^3cm^{-3}. Both the absolute errors of θ_s and θ_r of IPSO, GA and SA are equal or less than $0.006cm^3cm^{-3}$. The value of *RMSE* is the highest ($> 0.03459cm^3cm^{-3}$) for clay and the lowest ($< 0.00648cm^3cm^{-3}$) for silt loam. The R^2 and *RMSE* values of SA are the lowest and the highest among the three intelligent algorithms. For clay and clay loam, the sequences of values of both R^2 and *RMSE* from high to low and from low to high are all IPSO $>$ GA $>$ SA, respectively. The R^2 value in the estimation of VG equation parameters for silt loam by IPSO is equal to that by GA, and the *RMSE* value of IPSO is lower than that of GA. Both values of R^2 and *RMSE* of IPSO are the same with those of GA for sand loam. The R^2 and *RMSE* values in the determination of parameters of VG model for each soil texture by IPSO are the highest and lowest, respectively. All above results indicated that the parameter-optimization performance of IPSO is better than that of GA and SA.

5.2 Comparison of IPSO with RETC and Rosetta

The computer program RETC and PTF Rosetta are widely used to forecast SWRC in term of VG model. The nonlinear least square method is adopted in RETC and the initial values of VG equation parameters need to be set. Supposed that θ_r and θ_s are $0.1cm^3cm^{-3}$ and $0.5cm^3cm^{-3}$ respectively, α is $0.01cm^{-1}$, and n is 1.1 in this study. The water content calculated by IPSO, RETC (version 6.02) and Rosetta (version 1.2) were compared with those of measurement, see Figs.2-4.

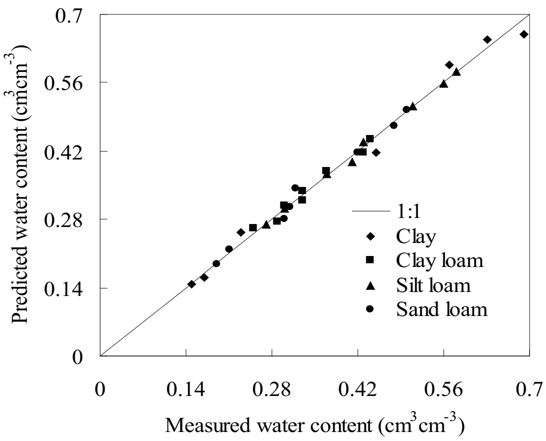

Fig. 2 Comparison of the predicted water content of IPSO with that of measurement [21] ($R^2 = 0.990$).

Table 4 showed the R^2 and *RMSE* values in determination of parameters of VG model by IPSO, RETC and Rosetta. It was found that the parameter of VG

Table 3 Parameters of VG model obtained from three intelligent algorithms and statistical analysis for simulation results

Soil texture	Intellgient algorithms	Parameters of VG model				Statistical analysis	
		θ_r/cm^3cm^{-3}	θ_s/cm^3cm^{-3}	α/cm^{-1}	n	R^2	$RMSE/10^{-2}cm^3cm^{-3}$
Clay	IPSO	0.154	0.600	0.103	2.365	0.981	3.459
	GA	0.160	0.600	0.096	2.649	0.979	3.487
	SA	0.158	0.600	0.095	2.825	0.977	3.596
Clay loam	IPSO	0.197	0.444	0.986	1.225	0.965	1.220
	GA	0.193	0.440	1.000	1.207	0.962	1.223
	SA	0.191	0.438	0.947	1.201	0.960	1.257
Silt loam	IPSO	0.200	0.585	0.535	1.272	0.997	0.618
	GA	0.200	0.581	0.484	1.276	0.997	0.627
	SA	0.195	0.581	0.532	1.259	0.996	0.648
Sand loam	IPSO	0.155	0.505	0.571	1.344	0.989	1.138
	GA	0.155	0.505	0.569	1.346	0.989	1.138
	SA	0.159	0.511	0.627	1.401	0.988	1.185

Table 4 Parameters of VG model obtained from three intelligent algorithms and statistical analysis for simulation results

Soil texture	Solution Methods	Parameters of VG model				Statistical analysis	
		θ_r/cm^3cm^{-3}	θ_s/cm^3cm^{-3}	α/cm^{-1}	n	R^2	$RMSE/10^{-2}cm^3cm^{-3}$
Clay	IPSO	0.142	0.659	0.180	1.850	0.988	2.211
	RETC	–	0.693	0.529	1.301	0.966	3.684
	Rosetta	0.065	0.490	0.055	1.442	0.702	10.963
Clay loam	IPSO	0.244	0.445	0.851	1.349	0.972	1.051
	RETC	0.244	0.445	0.849	1.349	0.972	1.051
	Rostta	0.136	0.413	0.053	1.321	0.588	4.020
Silt loam	IPSO	0.227	0.582	0.445	1.327	0.997	0.540
	RETC	–	0.588	1.114	1.115	0.985	1.293
	Rosetta	0.131	0.580	0.045	1.230	0.340	8.728
Sand loam	IPSO	0.155	0.505	0.569	1.346	0.989	1.138
	RETC	–	0.509	1.217	1.147	0.977	1.648
	Rosetta	0.076	0.487	0.031	1.274	0.529	9.558

Note: - indicates the parameter cannot be estimated.

equation of IPSO gives good results for the high R^2 value (> 0.97) and low *RMSE* value ($< 0.025cm^3cm^{-3}$). Fig. 3 showed that the predicted values by RETC are closed to the measured values ($R^2 = 0.974$). It is also supported by the value of R^2 from 0.966 to 0.985 and *RMSE* from 0.01051 to $0.03684cm^3cm^{-3}$ in Table 4. For clay loam, the value of R^2 and *RMSE* of RETC is identical with that of IPSO. However, for clay, silt loam and sand loam, the parameter θ_r could not be obtained by RETC, and the sequences of both R^2 values from high to low and *RMSE* from low to high are IPSO $>$ RETC $>$ Rosetta. It was found that the nonlinear least square method should be replaced by the method of IPSO to improve the accuracy of RETC in determination of the SWRC. For four soil textures, the value of R^2 and *RMSE* of Rosetta is the lowest (0.702, 0.588, 0.340 and 0.529) and highest (0.10963, 0.0402, 0.08728 and 0.09558 cm^3cm^{-3}), respectively. Fig. 4 showed that the results of Rosetta is not closed to the measured results ($R^2 = 0.585$). It was indicated that the Rosetta was not suitable to determine the SWRC for the agricultural soil textures studied here. Fig. 2 showed that the predicted results of IPSO are very close to the measured results. It was demonstrated that IPSO is reasonable and reliable to estimate the SWRC of VG model.

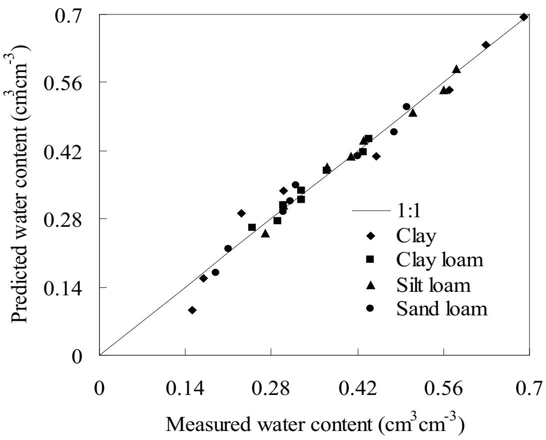

Fig. 3 Comparison of the predicted water content of RETC with that of measurement [21] ($R^2 = 0.974$).

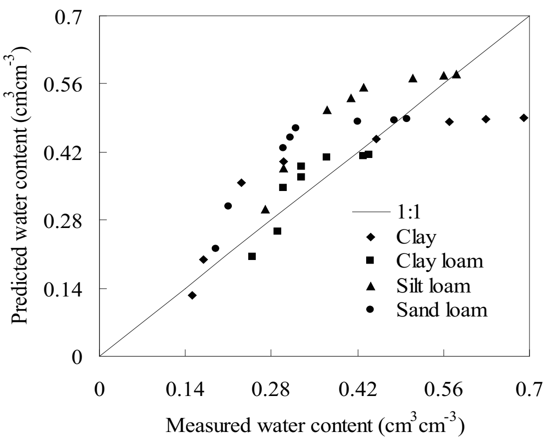

Fig. 4 Comparison of predicted water content of Rosetta with that of measurement [21] ($R^2 = 0.585$).

6 Conclusions

An improved particle swarm optimization (IPSO) was presented in this study. The intelligent algorithms such as IPSO, GA, and SA were used to determine parameters of VG model for the SWRC of four agricultural soil samples in China. The coefficient of determination (R^2) and root mean square error (*RMSE*) were used to quantify the differences between the predicted values and the measured values. The R^2 values for IPSO, GA and SA in the estimation of VG equation parameters are equal or greater than 0.960. The R^2 and *RMSE* values in the determination of parameters of VG model for four soil textures by IPSO are the highest and lowest, respectively. It indicated that the performance of parameter-optimization of IPSO is better than GA and SA.

The fitted results of IPSO were compared with those of RETC and Rosetta. The predicted values of water content of RETC are closed to the measured values ($R^2 = 0.974$). However, for clay, silt loam and sand loam, the parameter θ_r cannot be obtained by RETC at a given initial values of parameters. For the four soil textures, the value of R^2 and *RMSE* of Rosetta is the lowest and highest, respectively. The results of Rosetta are far away from the measured results ($R^2 = 0.585$). It was concluded that the method of Rosetta is not suitable to determine the SWRC of the four agricultural soil textures studied. The predicted results of IPSO are very closed to the measured results ($R^2 = 0.990$). It was demonstrated that IPSO is more reasonable and reliable to estimate the SWRC in term of VG model than the method of GA, SA, RETC and Rosetta. The method of IPSO improves the accuracy of parameters determination of VG model and the elimination of initial value influence and the avoidance of soil-column experiment are also realized in present study.

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