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An algorithm for the soil characteristic curve with the method of conjugate directions

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Abstract

A special algorithm is developed to optimize the function of van Genuchten, which is used for the simulation of the soil characteristic curve. This function is non-linear so the method of conjugate directions is used. A start point and a gradient are chosen and the next point is found by the optimum step size procedure (O.S.S.P.). The selected directions for the solution are found using the property of conjugate gradients and each direction is a function of the present and the last gradient.

1 Introduction

The unsaturated state of the soil is described by the soil water content θ (cm^3/cm^3) and the pore water pressure (suction) Ψ (cm). The relationship between these hydraulic parameters is called soil characteristic curve $\Psi(\theta)$ and is determined experimentally at the laboratory or at the field. This curve can be approximated by empirical prediction models, as Brooks & Corey[2], Brutsaert[3], Van Genuchten[11]. The most popular of the above functions is the equation of van Genuchten[11]:

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$$\frac{\theta-\theta_r}{\theta_s-\theta_r}=\frac{1}{\left[1+(\alpha\,\Psi)^n\right]^m}, \tag{1}$$

where θ is the soil-water content, θ_S is the soil-water content at saturation, θ_r is the residual soil-water content, Ψ is the pressure head of soil water (or suction in absolute value), a, n and m are empirical parameters which are estimated by fitting the experimental points with the equation of van Genuchten[11].

The above *simulation functions* are non-linear, so several algorithms have been developed to estimate their parameters. These algorithms are classified in the categories:

- Algorithms leading to the Gauss equations under linear transformation.
- Algorithms leading to linearized equations upon expanding the function in Taylor series, mentioned as Gauss or Gauss-Newton method.
- Algorithms which lead at direct solution of the non-linear problems, by using the steepest descent method.

In this paper a new optimisation algorithm is presented for the estimation of the parameters of van Genuchten[11] equation. This algorithm solves directly the non-linear equation and uses the method of *conjugate directions*.

2 Mathematics development

The method of conjugate directions is used to optimise a function *f*, under certain constrains. This method uses the property of conjugate vectors with respect to a matrix:

"A set of *n* linear independent non zero vectors $\vec{s}_k$, (k = 1, 2...n) is called conjugate with respect to a positive definite matrix $\boldsymbol{H}$ if:

$$\vec{s}_i^{\,T}\cdot\boldsymbol{H}\cdot\vec{s}_j=0 \quad \forall i, j\ or\ 1\le i\neq j\le n, \tag{2}$$

where the tensor $\boldsymbol{H}$ is Hessian matrix of function *f*, $(\boldsymbol{H}=\nabla(\nabla f(\vec{x}^k))$, where $\vec{x}^k=x_i\vec{e}_i$ is the position vector for the *k* point).

The most popular method of the *conjugate directions* is the method of *conjugate gradients,* proposed by Hesteness & Stiefel[5] and transformed by Fletcher & Reeves[6].

According to the above researchers this method is iterative and at the k step a direction $\vec{s}_k$ is derived, as a linear combination of $\nabla f(\vec{x}^k)$ and the previous directions $\vec{s}^a$, (a=1, 2...k-1).

The coefficients of linear combinations are chosen in such a way that the derived directions must be conjugate with respect to the Hessian matrix of the objective function f:

$$\vec{s}_i^T \cdot \boldsymbol{H} \cdot \vec{s}_j = 0. \tag{3}$$

Only the current gradient $\nabla f(\vec{x}^k)$ and the previous $\nabla f(\vec{x}^{k-1})$ are used for the estimation of these coefficients.

This method starts with an initial approach $\vec{x}^0$ and the steepest descent direction is chosen as the first direction of minimization:

$$\vec{s}^0 = -\nabla f(\vec{x}^0), \tag{4}$$

For the next point the following equation is chosen:

$$\vec{x}^1 = \vec{x}^0 + \lambda_0 \vec{s}^0, \tag{5}$$

where λ_0 is a parameter, obtained by the optimum step size procedure (O.S.S.P.).

The next direction $\vec{s}^1$ is obtained by the relationship:

$$\vec{s}^1 = -\nabla f(\vec{x}^1) + \omega_1 \vec{s}^0, \tag{6}$$

and it is a linear combination of $\nabla f(\vec{x}^1)$ and of the previous direction $\nabla f(\vec{x}^0)$.

The parameter ω_1 is chosen using the property of conjugate directions:

$$\vec{s}_1^T \cdot \boldsymbol{H} \cdot \vec{s}_0 = 0. \tag{7}$$

From this relationship it is obtained:

$$\omega_1 = \left\{ \frac{\left\| \nabla \vec{x}^1 \right\|}{\left\| \nabla \vec{x}^0 \right\|} \right\}^2 . \tag{8}$$

So the general algorithm is:

$$\vec{s}^k = -\nabla f(\vec{x}^k) + \omega_k \vec{s}^{k-1}, \tag{9}$$

$$\vec{x}^{k+1} = \vec{x}^k + \lambda_k \vec{s}^k, \tag{10}$$

and

$$\omega_k = \left\{ \frac{\left\| \nabla \vec{x}^k \right\|}{\left\| \nabla \vec{x}^{k-1} \right\|} \right\}^2 . \tag{11}$$

(the value of the step λ_k is estimated by the process of O.S.S.P.).
A criterion of convergence is examined in every step of iteration:

$$\left\|\vec{s}^{\,k}\right\| < \varepsilon, \text{ or } \left\|\nabla f(\vec{x}^{\,k})\right\| < \varepsilon, \tag{12}$$

where ε has a small value.
The minimized function *f* in the present problem is the following:

$$f = \sum_i \left\{\theta_i' - \theta_{i\,exp}\right\}^2, \tag{13}$$

where $\theta_i' = \theta_r + (\theta_s - \theta_r)/(1+(a\cdot\Psi)^n)^m$.

The parameters in the problem are:

- Two parameters model: *a, n (m=1-1/n).*
- Three parameters model: *a, n,* θ_r *(m=1-1/n).*

3 Conclusions

The soils, which were considered, are:

- Silt loam G.E.3 with θ_s=0.396 cm^3/cm^3 (van Genuchten[11])
- Medium sand of Thessaloniki with θ_s=0.350 cm^3/cm^3 (Sakellariou[7])
- Fine sand of Thessaloniki with θ_s=0.375 cm^3/cm^3 (Sismanis[10])
- Sand of N. Michaniona with θ_s=0.340 cm^3/cm^3 (Arampatzis[1]).

The results using the suggested model of conjugate directions are given in Figures 1-5. In the same Figures are also presented the results from other researchers which have used the linear model, the method of steepest decent, the method of Newton-Ramson and the method of Gauss (upon expanding the function in Taylor series). The value of parameters *a* and *n* for the case of two parameters model and *a*, *n* and θ_r for the case of three parameters model are given in Table 1. The results of convegence are given in Figure 6 (N.Michaniona's sand).

The suggested model of conjugate directions presents the minimum variance in comparison to the above methods. The coefficient of correlation is between 0.996 and 0.999 in all the cases.

Table 1

No (1)	Soil (authors) (2)	Model (3)	a (4)	n (5)	θ_r (6)	Variance (7)	R (8)
1	Silt loam G.E.3 (van Genucten[11])						
	Present algorithm	Conjugate dir.(2p)	0.004233	2.056596	0.1310	5.81E-06	0.99969
	Sakellariou[8]	Taylor(2p)	0.004232	2.056700	0.1310	6.64E-06	0.99900
	van Genuchten[11]	Steepest desc.(3p)	0.004233	2.059400	0.1313	6.65E-06	0.99900
	Sidir. & Giann.[9]	Newton-Raphson(2p	0.004233	2.059400	0.1310	6.70E-06	0.98561
2	Thessaloniki's medium sand (Sakellariou[7])						
	Present algorithm	Congugate dir.(2p)	0.055760	3.992726	0.1080	2.33E-05	0.99836
	Sakellariou[8]	Linear.(2p)	0.048500	4.604000	0.1080	3.61E-04	0.98560
3	Thessaloniki's fine sand (Sismanis[10])						
	Present algorithm	Congugate dir.(2p)	0.050281	2.759488	0.0630	4.04E-04	0.99856
	Sakellariou[8]	Taylor(2p)	0.049410	2.810640	0.0630	4.10E-04	0.99800
4	Thessaloniki's fine sand (Sismanis[10])						
	Present algorithm	Congugate dir.(3p)	0.050820	2.509923	0.04934	2.06E-05	0.99896
	Sakellariou[8]	Taylor(3p)	0.050810	2.509950	0.04900	2.19E-05	0.99800
5	N.Michaniona's sand (Arampatzis[1])						
	Present algorithm	Congugate dir.(2p)	0.073567	4.596102	0.0200	7.62E-05	0.99646
	Arampatzis[1]	Steepest desc.(2p)	0.073560	4.596360	0.0200	7.62E-05	0.99277

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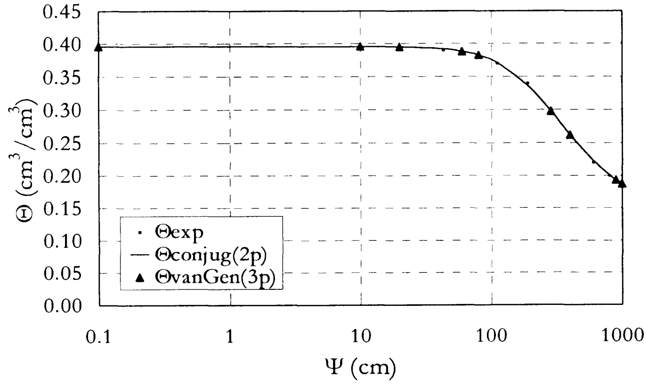

Figure 1. Characteristic curve *Ψ(θ)*. Silt loam G.E.3 (van Genuchten 1978).

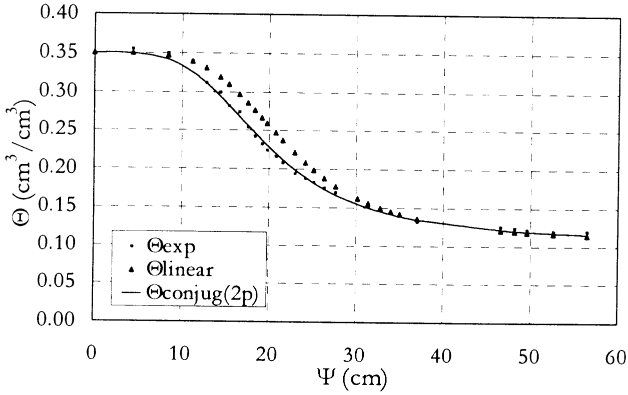

Figure 2 Characteristic curve $\Psi(\theta)$. Thessaloniki's medium sand (Sakellariou 1986).

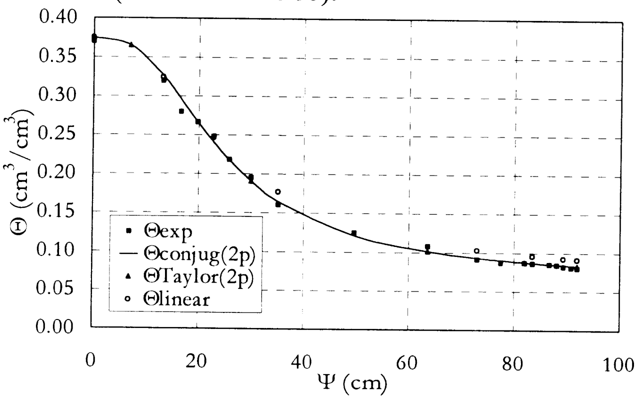

Figure 3. Characteristic curve $\Psi(\theta)$. Thessaloniki's fine sand (Sismanis 1992).

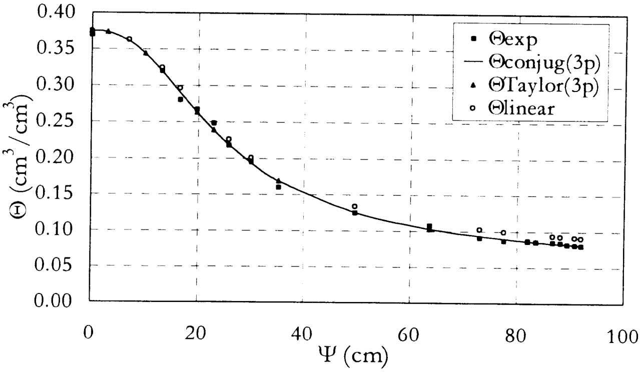

Figure 4. Characteristic curve $\Psi(\theta)$. Thessaloniki's fine sand (Sismanis 1992).

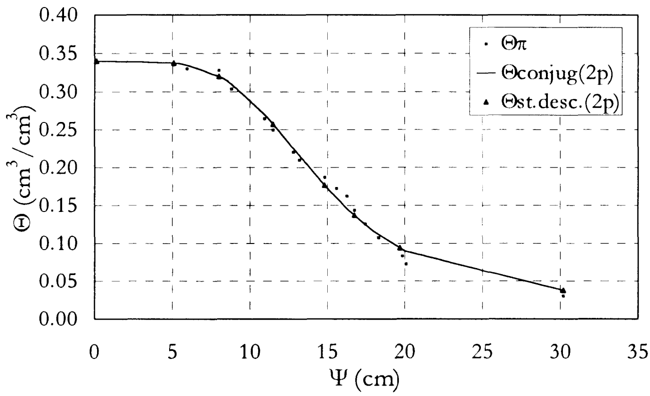

Figure 5. Characteristic curve $\Psi(\theta)$. N. Michaniona's sand (Arampatzis 1996).

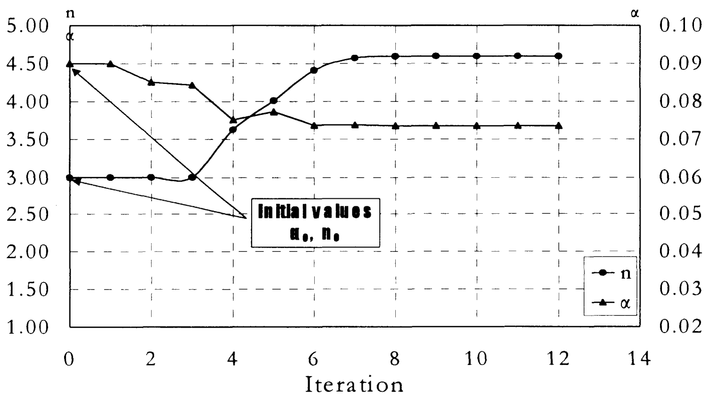

Figure 6. The convergence of a and n parameters, used the method of conjugate directions (Arampatzis 1996).