Determining Soil Parameters

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Content

- Problem Formulation
- Discretization of the Direct Problem
- Discrete Optimal Control Problem
- FAD Technique
- Computational Algorithm for Calculating Derivatives of the Objective Function
- Numerical Solution of the Problem
- Conclusions

Initial boundary value problem:

$$
\begin{aligned}
&\frac{\partial\theta}{\partial t} = \frac{\partial}{\partial z}\left(D(\theta)\frac{\partial\theta}{\partial z}\right) - \frac{\partial K(\theta)}{\partial z}, \quad (z,t) \in Q,\\
&\theta(z,0) = \varphi(z), \quad z \in (0, \mathrm{L}),\\
&\theta(L,t) = \psi(t), \quad t \in (0,T),\\
&-\left(D(\theta)\frac{\partial\theta}{\partial z} - K(\theta)\right)\Bigg|_{z=0} = R(t) - E(t), \quad t \in (0,T),\\
&\theta_{min} \le \theta(0,t) \le \theta_{max}, \quad t \in (0,T),
\end{aligned}
\qquad (1)
$$

$Q = (0,L) \times (0,T)$;
$D(\theta)$ and $K(\theta)$ are diffusion coefficient and hydraulic conductivity
$\theta_{min} = \theta_r + \varepsilon$, $\theta_{max} = \theta_s - \varepsilon$, $\quad 0 < \varepsilon \ll \theta_r$;
θ_r, θ_s are the residual moisture and the saturation moisture;
$R(t)$ is precipitation;
$E(t)$ is evaporation, $0 \le E(t) \le M$, $t \in (0,T)$, $M > 0$.

Van Genuchten formulas

$$K(\theta) = K_0 S^{0.5}[1 - (1 - S^{1/m})^m]^2,$$
$$D(\theta) = K_0 \frac{1-m}{\alpha m(\theta_s - \theta_r)} S^{0.5-1/m} \times [(1 - S^{1/m})^{-m} + (1 - S^{1/m})^m - 2], \quad (2)$$

$S = \dfrac{\theta - \theta_r}{\theta_s - \theta_r}$; θ_s is given constant;
K_0, α, m, θ_r are parameters.

A function $\hat{\theta}(z, t)$ is defined on some set $Q_0 \subseteq Q$.
Introduce a set
$U = \{u : u \in R^4;\ 0 \le a[i] \le u[i] \le b[i],\ i = 1, 2, 3, 4\}$
and denote $[K_0, \alpha, m, \theta_r]^\top$ by u.

Optimal Control Problem

The problem is to find u^{opt}, $u^{opt} \in U$, and the corresponding solution $\theta^{opt}(z, t)$ of the direct problem (1)-(2) which minimize functional

$$J = \frac{1}{2} \int_{Q_0} (\theta - \hat{\theta})^2 dzdt. \qquad (3)$$

Discretization of the Direct Problem

Divide $(0, T)$ and $(0, L)$ into N and I equal subinterval, $t^n = \tau n$, $0 \le n \le N$, $z_i = hi$, $0 \le i \le I$, $\tau = T/N$ and $h = L/I$.
Denote $\theta(ih, n\tau)$ by θ_i^n, $0 \le i \le I$, $0 \le n \le N$.
The direct problem is approximated by finite differences scheme:

$$\frac{\theta_i^{n+1} - \theta_i^n}{\tau} = \frac{1}{h}\left(D_{i+1/2}^{n+1}\frac{\theta_{i+1}^{n+1} - \theta_i^{n+1}}{h} - K_{i+1/2}^{n+1} - \right.$$
$$\left. - D_{i-1/2}^{n+1}\frac{\theta_i^{n+1} - \theta_{i-1}^{n+1}}{h} + K_{i-1/2}^{n+1}\right),$$
$$1 \le i < I; \quad 0 \le n < N,$$
$$\theta_i^0 = \varphi_i, \quad 0 \le i \le I, \quad \theta_I^n = \psi^n, \quad 1 \le n \le N,$$

$$D_{i-1/2}^n = D(\theta((i-1/2)h, n\tau), \quad K_{i-1/2}^n = K(\theta((i-1/2)h, n\tau),$$
$$1 \le i \le I; \ 1 \le n \le N.$$

The left boundary condition is discretized in the form

$$\frac{\theta_0^{n+1} - \theta_0^n}{\tau} = \frac{2}{h}\left(D_{1/2}^{n+1} \frac{\theta_1^{n+1} - \theta_0^{n+1}}{h} - \right.$$
$$\left. - K_{1/2}^{n+1} + R^{n+1} - E^{n+1} \right),$$
$$0 \leq n < N,$$

$$R^{n+1} = R((n+1)\tau), \quad E^{n+1} = E((n+1)\tau), \quad 0 \leq n < N.$$

$$
\begin{aligned}
&\Phi_0^n = -\left(\frac{1}{\tau} + \frac{2}{h} D_{1/2}^n\right)\theta_0^n + \frac{2}{h} D_{1/2}^n \theta_1^n \\
&+\frac{1}{\tau}\theta_0^{n-1} + \frac{2}{h}\left(-K_{1/2}^n + R^n - E^n\right) = 0, \\
&\theta_{min} \le \theta_0^n \le \theta_{max}, \quad 1 \le n \le N, \\
&\Phi_i^n = \frac{1}{h^2} D_{i-1/2}^n \theta_{i-1}^n + \frac{1}{h^2} D_{i+1/2}^n \theta_{i+1}^n - \\
&\left\{\frac{1}{\tau} + \frac{1}{h^2}\left(D_{i+1/2}^n + D_{i-1/2}^n\right)\right\}\theta_i^n + \\
&+\left\{\frac{\theta_i^{n-1}}{\tau} + \frac{1}{h}\left(K_{i-1/2}^n - K_{i+1/2}^n\right)\right\} = 0, \\
&\quad 1 \le i \le I-1, \quad 1 \le n \le N, \\
&\Phi_I^n = \theta_I^n - \psi^n = 0, \quad 1 \le n \le N, \\
&\theta_i^0 = \varphi_i, \quad 0 \le i \le I.
\end{aligned}
\tag{4}
$$

The diffusion coefficient and the hydraulic conductivity at the intermediate points:

$$D^n_{i+1/2} = \frac{D^{n-1}_i + D^{n-1}_{i+1}}{2}, \quad K^n_{i+1/2} = \frac{K^{n-1}_i + K^{n-1}_{i+1}}{2}, \tag{5}$$
$$1 \le n \le N, \quad 0 \le i < I.$$

Discrete Optimal Control Problem

Introduce a set :

$$Q_0 = \{(z, t) : z = ih, t = l\tau, (i, l) \in A\},$$
$$A = \{(i, l) : i = 0, 1, \dots, I, \ l = 1, \dots, d\}, 0 < d \leq N.$$

Define the objective function in the form

$$W(\theta, u) = \frac{1}{2} \sum_{(j,n) \in A} \left(\theta_j^n - \hat{\theta}_j^n \right)^2 \tau h, \tag{6}$$

where $\hat{\theta}_j^n = \hat{\theta}(jh, n\tau)$, $(j, n) \in A$.

Optimal Control Problem

The optimal control problem is to find optimal control $u^{opt} \in U$ and corresponding optimal solution $\theta^{opt}(z, t)$ of the direct problem (4)-(5) that minimize the objective function $W(\theta, u)$ (6).

FAD Technique

Let mappings $W : R^n \times R^r \to R^1$, $\Phi : R^n \times R^r \to R^n$ be twice continuously differentiable.
Let $x \in R^n$ and $u \in R^r$ satisfy the system of n scalar algebraic equations:

$$\Phi(x, u) = 0_n. \tag{7}$$

We introduce designations:

$$\Phi_x^{\top}(x, u) = \|a_{ij}\| = \|\partial \Phi^j / \partial x^i\|, \quad i = 1, 2, \ldots, n, \; j = 1, 2, \ldots, n,$$
$$\Phi_{x^{\top}} = (\Phi_x^{\top})^{\top}.$$

Let the matrix $\Phi_x^{\top}(x, u)$ be non-singular. Then according to the implicit function theorem, the relations (7) define function $x = x(u) \in C^2(u)$. The variable x will be considered as a phase variable, and u – as a control.

The gradient of the function $W(z(u), u)$ is calculated by formula:

$$dW(u)/du = W_u(x(u), u) + \Phi_u^\top(x(u), u)p. \quad (8)$$

The Lagrange multiplier $p \in R^n$ is determined from the following linear system of equations :

$$W_x(x(u), u) + \Phi_x^\top(x(u), u)p = 0_n. \quad (9)$$

Formula for second derivatives of the function W:

$$
\begin{gathered}
d^2W(u)/du^2 = \Lambda^\top(u) L_{xx}(x(u), u, p(u))\Lambda(u) + \\
L_{uu}(x(u), u, p(u)) + L_{xu}(x(u), u, p(u))\Lambda(u) + \\
\Lambda^\top(u) L_{ux}(x(u), u, p(u)), \\
L(x, u, p) = W(x, u) + p^\top \Phi(x, u).
\end{gathered}
\tag{10}
$$

The matrix Λ is determined from matrix equation:

$$
\Phi_{x^\top}\Lambda + \Phi_{u^\top} = 0_{nr}. \tag{11}
$$

This matrix equation is linear with respect to Λ and consists of r systems of n equations.
Each system has the same basic matrix $\Phi_{x^\top}$.

Computational Algorithm for Calculating Derivatives of the Objective Function

All formulas for the first and second derivatives of $D^n_{i+1/2}$ and $K^n_{i+1/2}$ with respect to θ and u were derived using Maple computer algebra system and MATLAB symbolic computation package.

The location of all nonzero block elements of $\Phi_\theta^\top$:

$$\Phi_\theta^\top = \begin{pmatrix} G_{11} & G_{12} & & & \\ & G_{22} & G_{23} & & \\ & & \ddots & \ddots & \\ & & & G_{kk} & G_{kN} \\ & & & & G_{NN} \end{pmatrix}, \quad k = N-1. \qquad (12)$$

Computational Algorithm for Calculating Derivatives of the Objective Function

The location of all nonzero elements in G_{ii}, $1 \le i \le N$:

$$G_{ii} = \begin{pmatrix} C_0 & B_0 & & & \\ A_1 & C_1 & B_1 & & \\ & \ddots & \ddots & \ddots & \\ & & A_k & C_k & 0 \\ & & & A_N & C_N \end{pmatrix}. \tag{13}$$

The location of all nonzero elements in G_{ij}, $j = i + 1$, $1 \le i < N$:

$$G_{ij} = \begin{pmatrix} 1/\tau & & & & \\ & 1/\tau & & & \\ & & \ddots & & \\ & & & 1/\tau & \\ & & & & 0 \end{pmatrix}. \tag{14}$$

Computational Algorithm for Calculating Derivatives of the Objective Function

Determining p

The system (9) is split into N subsystems. Moving from bottom to top we solve each of these subsystems separately.
These subsystem are solved using tridiagonal matrix algorithm.

Computing gradient

After determining p, the gradient of the function W is calculated by formula (8). The formula allows parallelization.

Relative cost

The ratio of gradient computation time to the function computation time (relative cost) was approximately equal to 1.

According to expert assessments, the relative cost when using the Adept package, which is one of the fastest, is 2.5–4.

Computational Algorithm for Calculating Derivatives of the Objective Function

Determining the matrix Λ

The matrix equation (11) is split into r systems of n equations. All these systems have the same basic matrix $\Phi_{\theta^\top} = (\Phi_\theta^\top)^\top$. Each of these systems is solved similarly to the system (9), but from top to bottom. Solving the matrix equation (11) allows parallelization.

Calculating second derivatives by the formula (10)

The sparseness of the matrices involved, their symmetry and repeatability of their elements were used to reduce the amount of computation. This allows not only to reduce the computational time but also to increase the precision of calculating the derivatives. Calculating the second derivatives admits parallelization.

Numerical Solution of the Problem

The values of input parameters:

$$L = 100(\text{cm}), \quad T = 1/96(\text{d}), \quad \theta_s = 0.5(\text{cm}^3/\text{cm}^3),$$
$$\varphi(z) = 0.3,\ z \in (0, L),\ \psi(t) = 0.3,\ t \in (0, T),\ \varepsilon = 10^{-8}$$
$$a = [0, 0.0005, 0.08, 0.03]^T, \quad b = [300, 0.4, 0.8, 0.09]^T.$$

A grid: $I = 100$, $N = 1$.

The first stage of calculations

The direct problem with the parameters $K_0^{true} = 100(\text{cm}/\text{d})$, $\alpha^{true} = 0.01$, $m^{true} = 0.2$ and $\theta_r = 0.05$ was solved.
Obtained solution was taken as a prescribed function $\hat{\theta}(z, t)$.

The second stage of calculations

The parameters identification problem was solved by Newton method. The step size in the chosen direction was determined using the procedure of one-dimensional optimization of the function determined by interpolation of the objective function by splines. Interpolation was done using 20 points. The problem was numerically solved with various initial approximations.

First, as an initial approximation we took the approximation $u^{init} = u^0$: $K_0^0 = 110$, $\alpha^0 = 0.011$, $m^0 = 0.22$ and $\theta_r^0 = 0.055$. It took 714 iterations to find a solution. Percentage error is 0.123%, 0.056%, 0.033%, 0.144% for K_0, α, m and θ_r respectively.

Initial approximations differ from u^0 only in the values of K_0.

Table 1: Results of the first series

Initial value	Errors (%)				Number of iterations
K_0	K_0	α	m	θ_r	
100	0.116	0.052	0.031	0.136	877
120	0.117	0.053	0.031	0.137	502
130	0.126	0.057	0.033	0.145	195
140	0.127	0.057	0.034	0.149	543
150	0.139	0.063	0.037	0.163	753
160	0.139	0.063	0.037	0.163	924
90	0.122	0.055	0.032	0.143	1070
80	0.114	0.052	0.030	0.134	1344
70	0.126	0.057	0.033	0.148	1512
60	0.125	0.057	0.033	0.147	1502
50	0.143	0.065	0.038	0.168	1455
40	0.122	0.055	0.032	0.143	4636

Initial approximations differ from u^0 only in the values of α

Table 2: Results of the second series

Initial value	Errors (%)				Number of iterations
α	K_0	α	m	θ_r	
0.010	0.119	0.054	0.032	0.140	1086
0.018	0.129	0.058	0.034	0.152	1199
0.020	0.123	0.056	0.033	0.145	786
0.025	0.127	0.057	0.034	0.149	2921
0.030	0.128	0.058	0.034	0.150	1900
0.035	0.129	0.058	0.034	0.152	3012
0.009	0.109	0.049	0.029	0.128	1180
0.008	0.122	0.055	0.032	0.144	1192
0.007	0.115	0.052	0.030	0.135	1112
0.006	0.133	0.060	0.035	0.156	374

Numerical Solution of the Problem

The second stage of calculations, the third series

Initial approximations differ from u^0 only in the values of m.

Table 3: Results of the third series

Initial value	Errors (%)				Number of iterations
m	K_0	α	m	θ_r	
0.200	0.145	0.065	0.038	0.170	1048
0.250	0.114	0.051	0.030	0.134	1334
0.310	0.131	0.059	0.035	0.154	2620
0.450	0.121	0.055	0.032	0.143	4184
0.500	0.125	0.057	0.033	0.147	4838
0.550	0.141	0.064	0.037	0.165	5224
0.600	0.134	0.061	0.036	0.157	5525
0.650	0.128	0.058	0.034	0.150	5667
0.700	0.129	0.058	0.034	0.152	5727
0.180	0.141	0.064	0.037	0.166	1402
0.150	0.123	0.056	0.033	0.145	3017
0.120	0.122	0.055	0.032	0.144	3900
0.100	0.104	0.047	0.028	0.122	3990
0.080	0.124	0.056	0.033	0.146	6511

Numerical Solution of the Problem

The second stage of calculations, the fourth series

Initial approximations differ from u^0 only in the values of θ_r.

Table 4: Results of the fourth series

Initial value	Errors (%)				Number of iterations
θ_r	K_0	α	m	θ_r	
0.055	0.123	0.056	0.033	0.144	714
0.060	0.126	0.057	0.033	0.148	963
0.065	0.127	0.057	0.034	0.149	1098
0.070	0.126	0.057	0.033	0.148	1192
0.075	0.117	0.053	0.031	0.138	1275
0.080	0.127	0.057	0.034	0.149	1358
0.045	0.247	0.112	0.066	0.293	158
0.040	0.122	0.055	0.032	0.143	608
0.030	0.123	0.055	0.033	0.144	1220
0.050	0.124	0.056	0.033	0.146	576

Conclusions

Analysis of the numerical results allows us to conclude that the proposed method makes it possible to determine the parameters with high precision from soil moisture data. It should be noted that we consider the case of accurate initial data.