Levenberg–Marquardt Method for Restoration of Layered Medium Key Parameters[1]

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Abstract - **We consider the model of the anomalous diffusion process layered media exhibiting memory. We use fractional calculus as a mathematical description of such media and state the boundary value problem for the partial differential equation in fractional derivatives. We define inverse problems as the restoration of the medium key parameters including the anomalous diffusion index that correlates with the fractional dimension of the medium. The numerical approach involves numerical simulations of the process and variational methods for inverse problems. We present the numerical solutions obtained by means of the Levenberg–Marquardt method and discuss the corresponding results.**

I. INTRODUCTION

The Levenberg–Marquardt method described in [1] is an efficient optimization method for inverse problems of different sorts. We apply this standard technique for restoration of layered medium key parameters in order to make sure that it is also applicable in the case of media exhibiting memory.

In this work we study the anomalous diffusion process in a layered medium where every layer can be characterized with its thermal diffusivity λ and anomalous diffusion index α. We consider a semi-infinite rod with a thermal source producing a temperature wave localized at the end of a rod. The temperature wave intensity is registered by a detector localized at the boundary of the rod at some distance from the source.

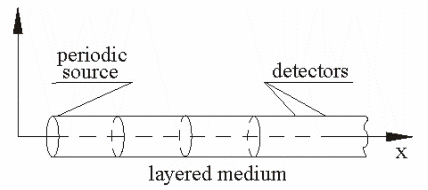

Fig. 1. The model under consideration

The efficient way of obtaining some information about a layered medium structure and makeup is to measure its temperature wave expose reaction as Fourier and Sommerfeld did before. The suggested technique allows us to restore the medium basic parameters with arbitrary accuracy. Notice that in this case we study the primary phase of temperature oscillation in order to solve inverse problems.

In the case of media exhibiting memory, application of Nigmatullin model gives rise to the following boundary value problem in $\Omega = \{(x,t) : x \geq 0, t \geq 0\}$:

$$\frac{\partial^\alpha u}{\partial t^\alpha} = \lambda^2 \frac{\partial^2 u}{\partial x^2}, \qquad 0 < \alpha < 2; \tag{1}$$

$$u(x,0) = 0, \ x \geq 0; \tag{2}$$

$$u_t(x,0) = 0, \ 1 < \alpha < 2, \ x \geq 0; \tag{3}$$

$$u(0,t) = f(t), \qquad u(+\infty,t) = 0, \qquad t \geq 0; \tag{4}$$

$$u(0,0) = f_0 = 0. \tag{5}$$

Here we use the Weyl fractional derivative of $u = u(x,t)$. We also assume that $\lambda = \lambda(x)$, $\alpha = \alpha(x)$ are step functions and $f(t)$ is the periodic function.

Sec. II suggests the variational approach to inverse problems. We define inverse problems as the optimization of the corresponding objective function and discuss the characteristics of this function according to its graphical representation. Besides, we formulate inverse problems and show that the existing iterative methods for standard coefficient inverse problems are also applicable in the case of inverse problems of anomalous diffusion.

Sec. III presents some numerical results and discusses their dependence on the source parameters. We use the Levenberg–Marquardt algorithm as the most effective technique that allows us to obtain the sought solution with arbitrary accuracy. We present the detailed description of the Levenberg–Marquardt algorithm and tabulate the results obtained by means of this technique.

II. VARIATIONAL APPROACH

The variational approach denotes the parameters to be varied according to the direct problem solution obtained.

We formulate inverse problems as the restoration of $\lambda = \lambda(x)$ and $\alpha = \alpha(x)$ according to the additional information about the solution

$$u(l,t) = \psi(t), \ 0 \leq t \leq T. \tag{6}$$

The detailed statements of the inverse problems to be considered in this section can be formulated as follows: according to (1)–(5) and (6) we need to determine

1) $\lambda(x)$ assuming $\alpha(x)$ to be a known variable;
2) $\alpha(x)$ assuming $\lambda(x)$ to be a known variable.

[1] Investigation partially supported by RFFI grants 05-01-00171, 05-01-00559 and grants SS-1172.2003.1, UR-04-01.200.

Mathematically, we can define inverse problem 2 as the restoration of the order of the corresponding partial differential equation.

The variational approach under consideration involves the inverse problem to be defined as the optimization of the residual function

$$\Psi\left[\chi(\mathrm{x})\right] = \int_0^T \eta(t;\chi(\mathrm{x}))^2\, dt = \int_0^T \left[\psi(t) - \xi(t;\chi(\mathrm{x}))\right]^2 dt\,, \quad (7)$$

where $\xi(t;\chi(\mathrm{x}))$ is the modeled data and $\chi(x)$ denotes $\alpha(x)$ or $\lambda(\mathrm{x})$.

The numerical investigations allowed us to understand the topography of the surface given by the residual function. In order to represent this surface graphically we consider its R^3-profile.

Fig. 2 and fig. 3 show that the topographic structure of the source given by the residual function is ravine and complex. The surface contains domains of local minima and in the case of $\alpha \neq 1$ the geometry of these domains is hypothesized to be self-similar. This fact denotes the correlation between the anomalous diffusion index and the fractional dimension of a medium exhibiting memory. The basic problem that needs to be solved is to use a method that would ignore the topographic structure of Ψ .

The minimum of the residual function (7) yields the solution for each of the inverse problems itemized above. In order to ignore local minima of the residual function

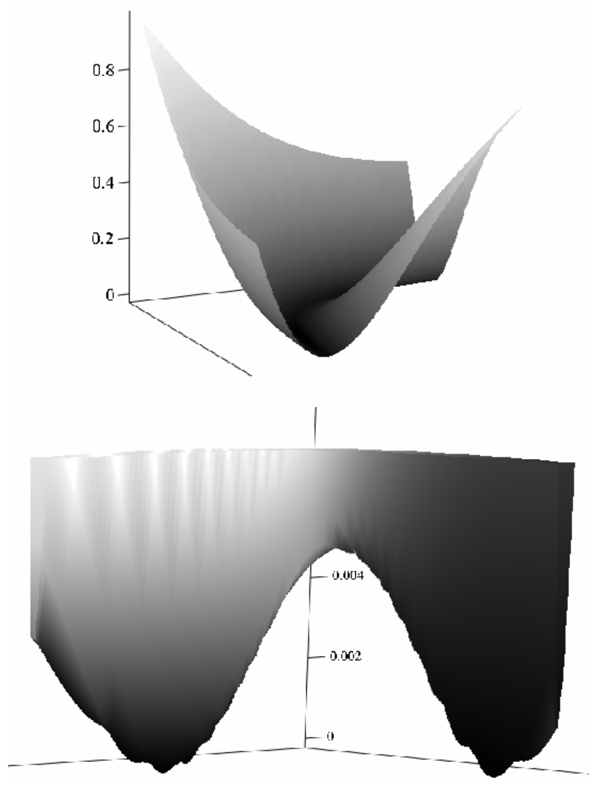

Fig. 2. The ravine surface of $\Psi(\lambda(\mathrm{x}))$ and its "bottom"

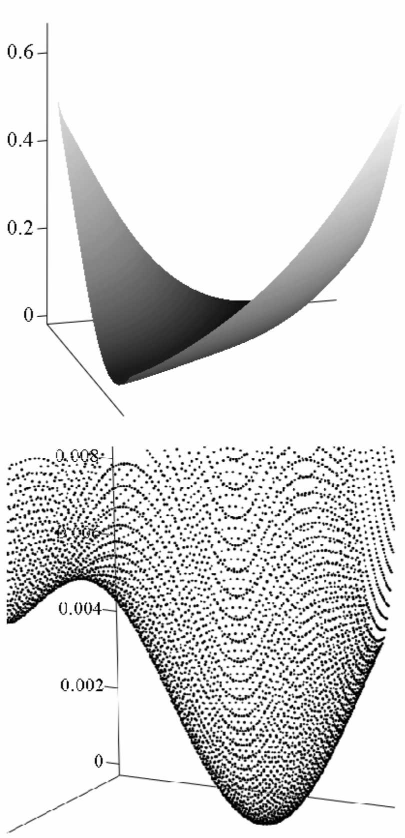

Fig. 3. The ravine surface of $\Psi(\alpha(\mathrm{x}))$ and its "bottom"

we choose Newton methods [2] with a linear step given by

$$\Delta\chi = -\left(\nabla^2\Psi(\chi)\right)^{-1}\nabla\Psi(\chi)\,. \quad (8)$$

The prototypical algorithm for Newton methods is the Levenberg–Marquardt algorithm described in [1]. The gradient $\nabla\Psi(\chi)$ can be represented as $\nabla\Psi(\chi) = \mathrm{J}^{\mathrm{T}}\eta$ where denotes the Jacobian. The Hessian $\mathrm{H} = \nabla^2\Psi(\chi)$ can be represented as $H = J^T J + \gamma I$ where γ is a non-dimensional fudge factor. Therefore we can represent (8) as follows

$$\Delta\chi = -\left(\mathrm{J}^{\mathrm{T}} J + \gamma I\right)^{-1} J^T \eta \quad (9)$$

or

$$\left(\mathrm{J}^{\mathrm{T}} J + \gamma I\right)\Delta\chi = -J^T\eta\,, \quad (10)$$

$$\chi^+ = \chi^c + \Delta\chi\,, \quad (11)$$

where χ^c denotes the current approximate solution and χ^+ denotes the next approximate solution of the corresponding inverse problem. Notice that the representation (10), (11) allows us to avoid matrix inversion while performing calculations.

Although the rate of convergence of the Levenberg–Marquardt algorithm is high, this method requires a lot of auxiliary calculations and computer time. In order to construct the Jacobian we use the finite-difference derivatives and have to solve the direct problem while constructing each column of the matrix. Besides, we solve the direct problem and evaluate $\Psi(\chi^+)$ in order to make sure that the necessary condition $\Psi(\chi^+) < \Psi(\chi^c)$ is valid. The algorithm under consideration repeats (10), (11) until $\Psi(\chi^+) < \varepsilon$.

The numerical experiments show that the variational approach allows us to obtain the solutions of inverse problems with arbitrary accuracy.

III. NUMERICAL EXPERIMENTS

See [3] for detailed discussion about the finite difference method of fractional order applied to perform the numerical solutions of the inverse problems itemized above.

In this section we present some numerical results obtained by means of the Levenberg–Marquardt algorithm.

1. *Define* ψ, $n = 0$, $\chi^{(0)}$, $\gamma^{(0)}$;
2. *Evaluate* $\Psi^{(0)}$:
   (a) *solve the direct problem and evaluate* $\xi\left(\chi^{(0)}\right)$;
   (b) $\eta\left(\chi^{(0)}\right) = \psi - \xi\left(\chi^{(0)}\right)$;
   (c) *evaluate* $s_1 = \Psi\left(\chi^{(0)}\right)$;
3. *Construct the Jacobian* $J_{ij} = \dfrac{\eta_i(\chi_j + \delta\chi) - \eta_i(\chi_j)}{\delta\chi}$;
4. *Evaluate the Newton step* $\Delta\chi$:
   (a) *evaluate* $J^T\eta$;
   (b) *evaluate* $J^T J + \gamma I$ *and apply (10);*
5. *Evaluate* $s_2 = \Psi(\chi + \Delta\chi)$;
6. *If* $s_2 < s_1$ *then*
   (a) $s_2 = s_1$, $\gamma = \gamma / c$, $c = const$;
   (b) $\chi = \chi + \Delta\chi$; $n = n + 1$; *go to 3;*
   else
   $\gamma = \gamma \cdot c$; *go to 4(b).*

In order to solve the stated inverse problems numerically we developed the program system. This program system corresponds to a family of Windows MFC Applications based on the system for interactive control of computing. This interactive system allows us to provide the dialog-mode calculations and control the process by making corrections of current conditions.

The program system also helped us to perform numerical simulations of the anomalous diffusion process and describe its behavior. The simulations were performed according to the principles of fractional calculus. We used the Grünwald–Letnikov fractional derivative as the difference approximation for the Weyl fractional derivative. The realization of the variational approach by means of this program system can be illustrated by the examples presented below.

The following selected examples prove that solutions of inverse problems itemized above depend on the source parameters. We choose $f(t) = A(1 + \cos(\omega t))$.

Inverse problem 1. We assume that $\alpha(x) = 1.7 \ \ \forall x$ and $\lambda^* = (0.4; 0.6; 0.5)^T$ is the sought solution. We choose $\lambda^0 = (0.45; 0.55; 0.55)^T$ as the null approximation and apply the iterative process (10), (11).

Fig. 4 contains the values of the residual function and the final approximate solution for $\varepsilon = 10^{-5}$.

$\omega = 0.2$, $A = 0.5$	
$\Psi^{(0)} = 3.639793 \cdot 10^{-1}$ $\Psi^{(1)} = 1.050789 \cdot 10^{-2}$ $\Psi^{(2)} = 5.030967 \cdot 10^{-3}$ $\Psi^{(3)} = 4.073980 \cdot 10^{-3}$ $\Psi^{(4)} = 1.030212 \cdot 10^{-3}$ $\Psi^{(5)} = 2.931176 \cdot 10^{-6}$	$\lambda_0^{(5)} = 0.400064$ $\lambda_1^{(5)} = 0.599723$ $\lambda_2^{(5)} = 0.500015$
$\omega = 0.2$, $A = 5$	
$\Psi^{(0)} = 3.084439 \cdot 10^{0}$ $\Psi^{(1)} = 4.629940 \cdot 10^{-1}$ $\Psi^{(2)} = 1.215780 \cdot 10^{-1}$ $\Psi^{(3)} = 3.551850 \cdot 10^{-4}$ $\Psi^{(4)} = 8.169301 \cdot 10^{-10}$	$\lambda_0^{(4)} = 0.400000$ $\lambda_1^{(4)} = 0.599999$ $\lambda_2^{(4)} = 0.500000$

Fig. 4. Solution of inverse problem 1

$\omega = 0.2$, $A = 1$	
$\Psi^{(0)} = 3.484664 \cdot 10^{-1}$ $\Psi^{(1)} = 6.999159 \cdot 10^{-3}$ $\Psi^{(2)} = 2.046974 \cdot 10^{-3}$ $\Psi^{(3)} = 9.611256 \cdot 10^{-4}$ $\Psi^{(4)} = 8.894475 \cdot 10^{-4}$ $\Psi^{(5)} = 8.357607 \cdot 10^{-4}$ $\Psi^{(6)} = 5.418346 \cdot 10^{-5}$ $\Psi^{(7)} = 1.083207 \cdot 10^{-7}$	$\alpha_0^{(7)} = 1.500105$ $\alpha_1^{(7)} = 1.599873$ $\alpha_2^{(7)} = 1.400006$
$\omega = 0.2$, $A = 5$	
$\Psi^{(0)} = 2.552618 \cdot 10^{-1}$ $\Psi^{(1)} = 3.946119 \cdot 10^{-2}$ $\Psi^{(2)} = 2.754273 \cdot 10^{-2}$ $\Psi^{(3)} = 1.135946 \cdot 10^{-2}$ $\Psi^{(4)} = 2.316281 \cdot 10^{-4}$ $\Psi^{(5)} = 7.220972 \cdot 10^{-8}$	$\alpha_0^{(5)} = 1.500018$ $\alpha_1^{(5)} = 1.599978$ $\alpha_2^{(5)} = 1.400001$

Fig. 5. Solution of inverse problem 2

Inverse problem 2. We assume that $\lambda(x) = 0.5 \quad \forall x$ and $\alpha^* = (1.5;1.6;1.4)^T$ is the sought solution. We choose $\lambda^0 = (1.55;1.55;1.45)^T$ as the null approximation and apply the iterative process (10), (11).

Fig. 4 contains the values of the residual function and the final approximate solution for $\varepsilon = 10^{-5}$.

Numerical experiments show that solutions of inverse problems almost do not depend on frequency ω but do depend on amplitude A.

IV. CONCLUSION

The results obtained illustrate that the Levenberg–Marquardt method is applicable and efficient in the case of media exhibiting memory. Its rate of convergence is high and its domain of convergence is wide enough to successfully use it in practice.

The ulterior investigations will consist in

1) restoring $\lambda(x)$ and $\alpha(x)$ simultaneously;

2) extending one-dimensional case to three-dimensional case.

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