COMPUTATIONAL IDENTIFICATION OF THE MINOR COEFFICIENT OF THE ANOMALOUS SUBDIFFUSION EQUATION

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Dedicated to 75-th birthday of Vasiliy Ivanovich Vasil'ev

Abstract: The article is devoted to the numerical solution of the nonlinear inverse problem of identifying the time-dependent junior coefficient of the differential equation of anomalous diffusion. The overdetermination condition is specified $\forall t \in (0, T]$ as a function value at an interior point of the domain, or as an integral of the solution over a spatial domain or part of it. An implicit difference scheme is constructed using the finite difference method. We close it with a discrete analog of the overdetermination condition, and as a result, we obtain a nonlinear system of algebraic equations. For its numerical implementation at each time layer, a non-iteration method based on decomposition into two systems of linear algebraic equations with a tridiagonal matrix is proposed. The results of the computational experiment on test problems showed a fairly high accuracy of the proposed method.

Keywords: Caputo fractional time derivative, anomalous diffusion equation, coefficient inverse problem, finite difference method, implicit difference scheme, decomposition method, computational experiment.

1 Introduction

Inverse problems for differential and integro-differential equations, due to their numerous applications, attract the attention of many researchers. The formulation, theoretical issues of proving conditional correctness, the construction of computational methods for their numerical and various applications are summarized in the monographs [1] – [5].

The article [6] considers the inverse problem of determining the time-dependent coefficient of the right-hand side of a parabolic equation with an overdetermination condition at an interior point of the domain. An implicit difference scheme is constructed, its convergence is proven, and the results of the numerical solution are presented. In the cycle of works [7] – [10], effective non-iterative numerical methods for solving inverse problems of identifying the time-dependent junior coefficient of a parabolic equation are proposed. Time-dependent local and non-local overdetermination conditions were specified as the overdetermination condition.

The breadth of the application area in modeling various processes, a more accurate description of the process under study, corresponding to the order of the fractional time derivative are certainly attractive to researchers. In the work [11], schemes for the numerical solution of initial-boundary value problems for the anomalous diffusion equation are constructed using finite difference and finite element methods. The authors present numerical examples demonstrating the computational efficiency of the proposed method. The article [12] is devoted to the construction of an implicit difference approximation of the fractional Caputo derivative with respect to time for the anomalous diffusion equation. The authors proved its stability and convergence, and presented numerical examples demonstrating the computational efficiency of the proposed method. In the work [13], an implicit unconditionally stable numerical method is proposed for solving a one-dimensional linear fractional subdiffusion equation. Several examples of numerical implementation are presented. The article [14] is devoted to the numerical solution of the nonlocal equation of fractional diffusion with respect to time. The results of numerical calculations on test examples are presented, confirming the theoretical results. In the article [15] the uniqueness and existence of solutions of the anomalous diffusion equation are proved. In the work [16] an analytical algorithm for nonlinear equations with fractional derivative with respect to time is proposed. Examples of solving initial-boundary value problems for generalized Fisher equations with fractional derivative with respect to time are given. In the work [17] a new difference analog of the fractional Caputo derivative is proposed. On its basis difference schemes of a higher order of accuracy for the equation of anomalous diffusion with variable coefficients are constructed and theoretically substantiated. The presented numerical results have shown the efficiency of the proposed difference schemes.

In the paper [18] the boundary element method in combination with the generalized Tikhonov regularization is proposed for the numerical solution of

the inverse problem of determining the coefficient entering into the fractional diffusion equation. In the paper [19] the problem of determining the time-dependent convective transfer coefficient in the one-dimensional diffusion equation with a fractional time derivative is considered. Its correctness is proved. An efficient computational algorithm is developed for its numerical solution. In the paper [20] an analogue of the Crank-Nicolson difference scheme is proposed for the numerical solution of the initial-boundary value problem for the Grunwald-Letnikov differential heat conduction equation with a fractional time derivative. The results of a computational experiment are presented. In the paper [21] the L1/LDG method with alternating flows for solving the generalized Burgers equation with a fractional time derivative is numerically investigated. Numerical calculations confirmed the obtained theoretical results. In the article [22] an iterative method for identifying the order of the fractional time derivative for the anomalous diffusion equation is proposed. Numerical calculations on model problems with exact solutions have shown the effectiveness of the method. In the article [23] a new fractional derivative based on the Lagrange approach is proposed. For the numerical solution of the one-dimensional diffusion-convection equation with the introduced fractional derivative, a difference scheme on moving grids is constructed and theoretically justified.

In this paper, a method for numerically solving a nonlinear inverse problem of identifying the linear runoff coefficient under given redefinition conditions is proposed. An implicit scheme is constructed that approximates the problem. During its numerical implementation, at each time layer, the desired system of algebraic equations is split into two linear systems with the same matrix by applying a special decomposition. And the desired runoff coefficient is determined from a discrete analogue of the redefinition condition.

2   problem statement

Consider a nonlinear inverse initial-boundary value problem for a linear one-dimensional anomalous diffusion equation with a fractional Caputo time derivative of order $\alpha \in (0,1)$ and a linear sink with an unknown time-dependent coefficient, satisfying given inhomogeneous initial and Dirichlet boundary conditions. Suppose that the overriding condition is set to the value of the desired function at an interior point for $t \in (0,T]$. Thus, it is required to determine a pair of functions $u(x,t)$ and $p(t)$ from the conditions:

$$\begin{cases} \dfrac{\partial^\alpha u}{\partial t^\alpha} = \dfrac{\partial^2 u}{\partial x^2} - p(t)u(x,t), & 0 < x < l, \qquad 0 < t \leqslant T, \\[2mm] u(0,t) = \mu_1(t), \quad u(l,t) = \mu_2(t), \qquad 0 < t \leqslant T, \\[2mm] u(x,0) = \varphi(x), \qquad 0 \leqslant x \leqslant l, \qquad p(0) = p_0, \\[2mm] u(x^*,t) = \phi(t), \qquad 0 < t \leqslant T, \end{cases} \qquad (1)$$

where is a fixed point $x^* \in (0, l)$.

The fractional Caputo derivative of order α is defined by the formula:

$$\frac{\partial^\alpha u(x,t)}{\partial t^\alpha} = \frac{1}{\Gamma(1-\alpha)} \int\limits_0^t \frac{\partial u(x,s)ds}{\partial t}(t-s)^{-\alpha}. \qquad (2)$$

where $\alpha \in (0,1)$, $\Gamma(\cdot)$ is the gamma function.

3   Building the difference scheme

In the domain of definition $[0,l] \times [0,T]$ of the problem (1), we introduce a rectangular uniform grid in the spatial variable and time

$$\overline{\omega}_h = \{x_i = ih, \ i = 0,1,\dots,N; \ h = l/N; \ x^* = nh\},$$

$$\overline{\omega}_\tau = \{t_m = m\tau, \ m = 0,1,\dots,M; \ \tau = T/M\}, \quad \overline{\omega}_{h\tau} = \overline{\omega}_h \times \overline{\omega}_\tau.$$

In the differential equation of anomalous diffusion (1), to approximate the nonlocal fractional Caputo derivative of order α on the time layer $t = t_{m+1}$, we use the expression first proposed by P. Zhuang and F. Liu [12]:

$$\frac{\partial^\alpha u(x_i, t_{m+1})}{\partial t^\alpha} \approx \sigma_{\tau\alpha}\Big(-u_i^0 + \sum_{j=1}^m c_j u_i^{m-j+1} \Big), \quad m = 0,1,\dots,M-1, \quad (3)$$

where

$$\begin{cases} b_j = (j+1)^{1-\alpha} - j^{1-\alpha}, \quad j = 0,1,2\dots,m; \\ \\ c_j = b_{j-1} - b_j, \quad j = 1,2,\dots,m; \quad \sigma_{\tau\alpha} = \dfrac{1}{\Gamma(2-\alpha)\tau^\alpha}. \end{cases} \qquad (4)$$

They also showed that the approximation error of the fractional Caputo derivative is of the order of $O(\tau^{2-\alpha})$.

We will associate the inverse problem for the anomalous diffusion equation (1) with an implicit difference scheme, in which the linear sink is approximated with the second order in time $p(t_{m+0.5})u(x_i, t_{m+0.5}) = 0.5(p^{m+1}u_i^m + p^m u_i^{m+1})$, thus the discrete analogue of the subdiffusion equation takes the form:

$$\begin{cases} \sigma_{\tau\alpha}\Big(u_i^{m+1} - u_i^m + \sum_{j=2}^m s_j(u_i^{m-j+1} - u_i^{m-j}) \Big) = \\ \\ \dfrac{u_{i+1}^{m+1} - 2u_i^{m+1} + u_{i-1}^{m+1}}{h^2} - \big(p^{m+1}u_i^m + p^m u_i^{m+1}\big)/2, \\ \\ \qquad i = 1,2,\dots,N-1; \quad m = 0,1,\dots,M-1. \end{cases} \qquad (5)$$

We close the system of difference equations (5) with discrete analogs of the boundary and initial conditions, as well as the overdetermination condition:

$$\begin{cases} u_0^{m+1} = \mu_1^{m+1}, \quad u_N^{m+1} = \mu_2^{m+1}, \quad m = 0, 1, \ldots, M-1, \\[2mm] u_i^0 = \varphi_i, \quad i = 0, 1, \ldots, N; \quad p^0 = p_0, \\[2mm] u_n^{m+1} = \phi(t^{m+1}), \quad m = 0, 1, \ldots, M-1. \end{cases} \quad (6)$$

Now we describe the computational algorithm for the transition from the $m-$ th time layer to the next $m+1-$ th time layer, using the notations $r = h^2 \sigma_{\tau\alpha}$ and $\Psi = \sum_{j=0}^m c_j u_i^{m-j}$ in the system of equations (5) we obtain:

$$\begin{cases} ru_i^{m+1} = u_{i+1}^{m+1} - 2u_i^{m+1} + u_{i-1}^{m+1} + r\Psi - \dfrac{h^2}{2}(p^{m+1}u_i^m + p^m u_i^{m+1}), \\[3mm] \quad i = 1, 2, \ldots, N-1; \quad u_0^{m+1} = \mu_1^{m+1}, \quad u_N^{m+1} = \mu_2^{m+1}. \end{cases} \quad (7)$$

We rewrite the system of equations (7) in countable form:

$$\begin{cases} u_{i+1}^{m+1} - (r + 2 + h^2 p^m/2)u_i^{m+1} + u_{i-1}^{m+1} + r\Psi - h^2 p^{m+1}u_i^m/2 = 0, \\[3mm] \quad i = 1, 2, \ldots, N-1; \quad u_0^{m+1} = \mu_1^{m+1}, \quad u_N^{m+1} = \mu_2^{m+1}. \end{cases} \quad (8)$$

Using the decomposition method [7] we will seek the solution of the system of equations (8) in the form:

$$u_i^{m+1} = v_i + p^{m+1}w_i, \qquad i = 0, 1, \ldots, N, \quad (9)$$

and assuming that a sufficient condition for the sum to be zero is that the terms are zero, we obtain a system of equations:

$$\begin{cases} v_{i+1} - (r + 2 + h^2 p^m/2)v_i + v_{i-1} + r\Psi = 0, \\[3mm] w_{i+1} - (r + 2 + h^2 p^m/2))w_i + w_{i-1} - h^2 u_i^m/2 = 0, \\[3mm] i = 1, 2, \ldots, N-1; \; v_0 = \mu_1^{m+1}, \; w_N = \mu_2^{m+1}, \; v_0 = 0, \; w_N = 0. \end{cases} \quad (10)$$

Thus, the auxiliary grid functions v_i, w_i, $i = 0, 1, \ldots, N$ are calculated from the systems of linear algebraic equations (10).

From the overdetermination condition $u(x^*, t_{m+1}) = \phi(t_{m+1})$ we find

$$p^{m+1} = \frac{\phi^{m+1} - v_n^{m+1}}{w_n^{m+1}}. \quad (11)$$

The grid function u_i^{m+1} is determined by formula (9).

If the integral overdetermination condition (2) is given, then for an approximate calculation of the definite integral using the rectangle quadrature formula, we have:

$$p^{m+1} = \left(\phi^{m+1} - \sum_{i=0}^N v_i^{m+1}\hbar_i\right) \Big/ \left(\sum_{i=0}^N w_i^{m+1}\hbar_i\right), \quad (12)$$

where

$$\hbar_i = \begin{cases} h/2 & \text{for} \quad i = 0, N, \\ h & \text{otherwise.} \end{cases}$$

4   Computational experiment

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We present the results of the numerical implementation of the computational algorithm presented in the article on model problems with different values of the fractional time derivative exponent α, different initial conditions and override conditions.

Example 1. First, we solve the direct problem with known initial runoff coefficients:

$$\begin{cases} \dfrac{\partial^\alpha u}{\partial t^\alpha} = \dfrac{\partial^2 u}{\partial x^2} - p(t)u(x,t), & 0 < x < l, \qquad 0 < t \leqslant T, \\[2mm] u(x,0) = \dfrac{4x(l-x)}{l^2}e^{-(x-\frac{l}{2})^2}, & 0 \leqslant x \leqslant l, \\[2mm] u(0,t) = u(l,t) = 0, & 0 < t \leqslant T, \\[2mm] p(t) = e^{-100(t-0.5*T)^2}, & 0 \leqslant t \leqslant T. \end{cases} \qquad (13)$$

Let's start solving the coefficient inverse problem. Let's imagine that the coefficient $p(t)$ is not specified. Then, as the overdetermination condition, it is advisable to set $\phi^{m+1} = u_n^{m+1}$ – the values of the numerical solution of the direct problem (13) at the spatial grid node and u_n^{m+1}, $m = 1, 2, \ldots, M-1$.

It should be noted that the overdetermination condition is calculated as a result of solving the direct problem and therefore includes some noise, such as approximation error and inevitable computational rounding errors. Nevertheless, we will also conduct the experiment with artificial introduction of noise into the original data.

The solution of the problem (13) is carried out for different values of the order of the fractional derivative $\alpha = 0.1, 0.5, 0.9$ and for $x^* = x_{N/2}$. In Fig. 1, on the top left, the graphs of the solution at the final time for different values of the order of the fractional derivative with respect to time $u(x, T)$ and the initial condition $u(x, 0)$ are shown, and on the right, the graph of $p(t)$. On the bottom left, the graph of the difference between the solution of the direct problem and the solution of the inverse problem, and on the right, the error in determining $p(t)$ for different α. The calculations are carried out for $l = 20, T = 1, N = 100, M = 200$. The insignificant difference between the presented solutions of the direct and inverse problems for different values of the order of the fractional derivative with respect to time shows the high accuracy of the proposed non-iterative method for solving the posed inverse problem.
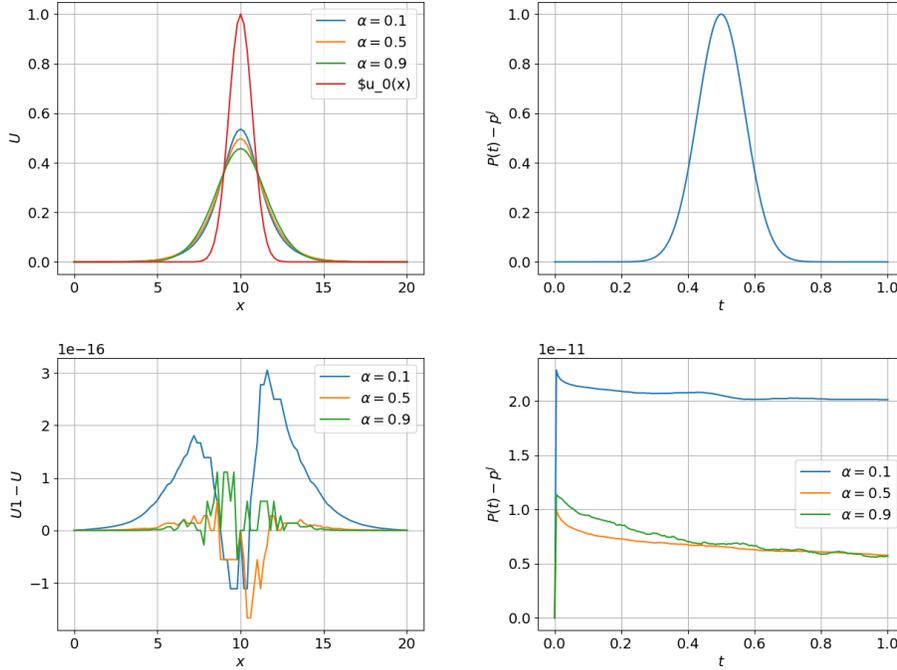
Fig. 1. Graphs of the numerical solution of the direct problem and the error in solving the inverse problem for different α at $x^* = l/2$
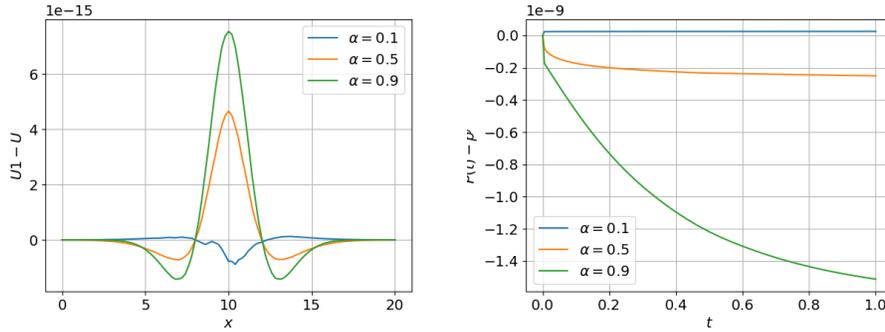

Fig. 2 Graphs of the error in determining the solution of the inverse problem for different α at $x^* = 0.4l$

Figure 2 shows the results of solving the inverse problem of determining the coefficient $p(t)$ for $x^* = x_{40}$. Shifting the selection point from the center for the overdetermination condition does not significantly worsen the accuracy.

Now consider the assignment of a non-local condition in the form of an integral $\phi(t) = \int_0^l u(x,t)dx$. The unknown coefficient at each time layer is determined using formula (12). Figure 3 shows the result when an additional
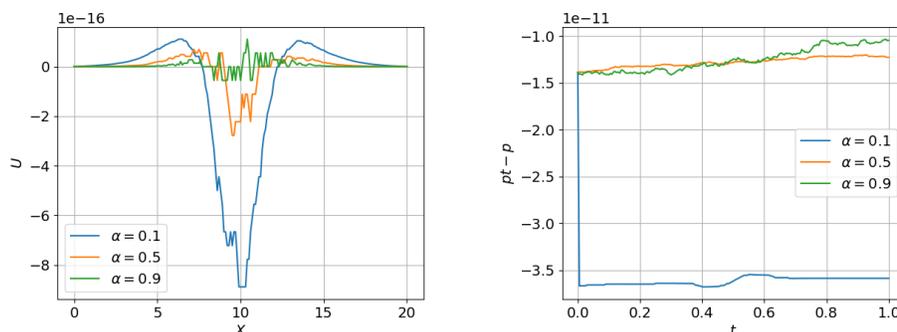
Fig. 3. Graphs of the error in determining the solution of the inverse
problem for different $\alpha =$ when setting the non-local overdetermination
condition

condition is specified as an integral over the domain for different orders
of the fractional derivative with respect to Caputo time. The accuracy of
the numerical solution is almost the same as with an additional condition
specified in the middle of the domain.

Example 2. In the following example, we define the runoff coefficient
$p(t)$, which is a discontinuous function of time:

$$p(t) = \begin{cases} 0, & 0 \leqslant t < T/3 \quad \& \quad 2T/3 < t \leqslant T, \\ 1, & T/3 \leqslant t \leqslant 2T/3. \end{cases} \tag{14}$$

We define the nonlocal overdetermination condition as the integral $\phi(t) = \int_0^l u(x,t)dx$, $t \in (0,T]$, $p(0) = 0$. First, we solve the direct problem (1). Then,
we proceed to the numerical solution of the inverse problem. At each time
layer, we define the overdetermination condition as $\phi^{m+1} = \sum_{i=0}^N u_i^{m+1}\hbar_i$.

The results of the numerical calculations are shown in Fig. 4, they confirmed
the high accuracy of the presented computational algorithm. It is evident
from the figure that the errors of both functions are minimal for all three
values of the order of the fractional derivative with respect to Caputo time.

Figure 5 shows the error graphs for different α, with artificial noise introduced
from the Python library
$noise = np.random.normal(0, 0.001, M)$ - random number generator uniformly
distributed in the segment $[0, 0.001]$. From the presented results it is evident
that at $\alpha = 0.9$ the error in determining the coefficient $p(t)$ is quite large.

5   Conclusion

For the numerical implementation of the finite-difference analogue of the
nonlocal inverse problem of determining the junior coefficient of the anomalous
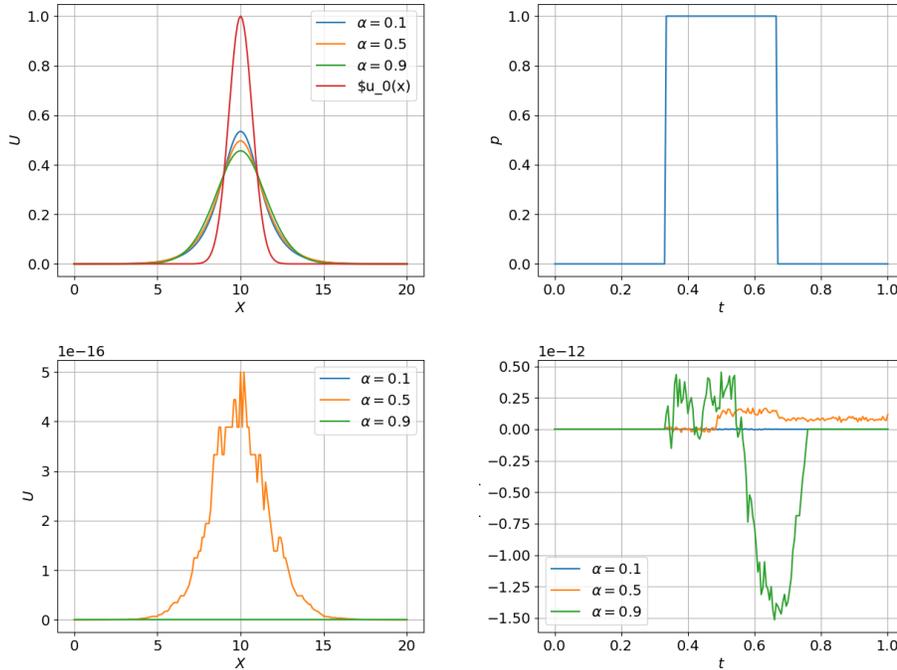
Fig. 4. Graphs of the numerical solution of the direct problem and the errors in determining the solution of the inverse problem for different α with a discontinuous coefficient (14)
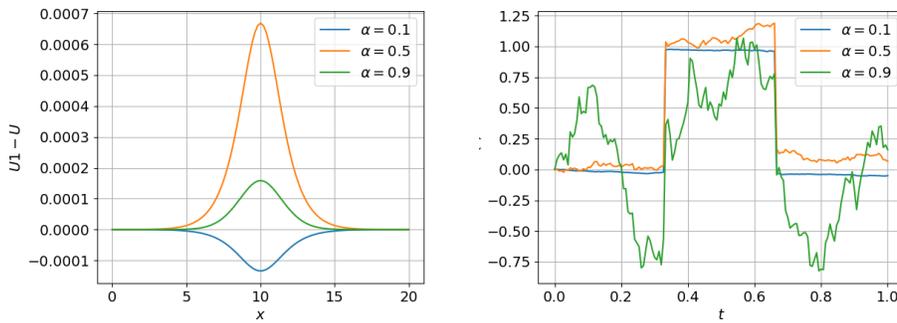

Fig. 5. Calculation results with noise introduced in the override condition

diffusion equation at each time layer, the decomposition method proposed in [7] is used, which allows obtaining two systems of linear algebraic equations with the same tridiagonal matrix. The results of the numerical implementation of the proposed computational algorithm are presented on model examples for different orders of fractional time derivative. The calculations showed a fairly high efficiency of the proposed method for numerically solving the coefficient inverse problem for the anomalous diffusion equation. It should be

noted that due to the conditional correctness of the original problem, a high sensitivity of the solution to the noise of the overdetermination condition is observed.

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