Fractional derivative order with respect to time for diffusion equation: an iterative method of determination

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Abstract. The article proposes the iterative method for the inverse problem that determines an $\alpha$-order of fractional derivative with respect to time for diffusion equation. The author presents the results obtained through numerical implementation of the method. The calculations were performed on model problems with exact solutions.

1. Introduction
In recent years, studies in the field of correctness and development of numerical methods for solving initial-boundary value problems for partial differential equations containing fractional derivatives have become extremely up-to-date. This is explained by their wide use as mathematical models for various natural phenomena and technological processes. Moreover, unlike classical derivative of integral order, there are many non-identical definitions for derivative of fractional order [1] – [4]. That leads to a variety of differential equations of fractional order that are similar in form, but significantly different in properties. In the middle of the 20th century, F. Mainardi and M. Caputo showed that differential equations with fractional derivatives for constructing thermoviscous elastic models were physically more accurate in reproducing experimentally observed data. A significant number of real processes does not fit into the concepts of continuum mechanics and require better information and idea about medium fractality in which they occur. The processes, for example, include impurity diffusion in liquids in highly porous media. In order to describe such processes one can use the modified Fick law [5], which requires an involvement of mathematical tools of fractional integro-differential calculus [6]. One introduces fractional derivatives with respect to spatial variables and time into a classical diffusion equation. Initial boundary value problems arise for differential equations with fractional derivatives (integro-differential equations). We see development of correctness studies for problems formulation, analytical methods for problems calculation. However, numerical methods became more popular in relation with their practical application. Primarily, this is due to the fact that analytical solutions can be obtained only in rare and special cases.

One can see an application of fractional partial derivatives in numerical solution of problems in the field of fluid mechanics and viscoplastic flow in [7], self-similar and multiscale structures in [8], the spatial Fokker-Planck fractional equation (SFFPE) with an instant source in [9], solutions of one-dimensional fractional advection-dispersion equations in work [10]. In the mentioned
studies, one can find numerous references to applications of fractional derivatives related to problems of Physics, Finance, and Hydrology.

When the fractional derivative replaces the first-order partial time derivative in the diffusion model, this leads to a slower diffusion (also known as sub-diffusion). In work [11], the finite sinusoidal transformation method is used to transform equations with fractional derivatives from the spatial domain to the wave number domain. Works [12], [13] study finite-difference schemes with adaptive regularization including mitigation methods. Article [14] discusses calculation of the Mittag-Leffler (ML) function with matrix arguments to construct solutions in the form of a series of trigonometric functions. Work [15] suggests the finite difference method for numerical calculation of the problem using the Grunwald-Letnikov definition for fractional time derivative. Another significant issue is an adequate determination of the fractional derivative index. Work [16] shows an inverse problem determining an order of the fractional derivative and a kernel through time measurements data. Work [17] offers identification of fractional orders in diffusion equations with multiple fractional time derivatives. In [18] derivative indicators order is determined through asymptotic behavior of their solutions. The studies are relevant indeed, since the index of the fractional derivative is determined by real physical properties of these materials.

The present work studies an inverse problem with respect to exponent of the fractional derivative. The author suggests an iterative secant method for numerical solution of the discrete analogue of the problem considered. Moreover, we can see a numerical solution of the direct problem at every iteration.

2. Statement of the problem

We consider the simplest one-dimensional differential equation with fractional time derivative with homogeneous boundary and inhomogeneous initial conditions. Let us set a measuring result of the function value inside the region at a finite moment in time as an additional condition. Thus, we consider an inverse problem that determines \( \alpha \in (0, 1) \) of the fractional time derivative:

\[
\begin{align*}
\frac{\partial^\alpha u}{\partial t^\alpha} &= \frac{\partial^2 u}{\partial x^2}, \\
0 < x < l, \quad 0 < t \leq T, \\
u(0, t) &= u(l, t) = 0, \quad 0 < t \leq T, \\
u(x, 0) &= \varphi(x), \quad 0 \leq x \leq l,
\end{align*}
\]

We set an additional condition in the following form

\[ u(\xi, T) = d, \quad \xi \in (0, 1). \]

where \( \xi \in (0, 1) \).

In equation (1) we take the Caputo fractional derivative of order \( \alpha \), as the fractional time derivative, determined by the formula:

\[
\frac{\partial^\alpha u(x, t)}{\partial t^\alpha} = \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{\partial u(x, s)}{\partial t}(t-s)^{-\alpha} ds,
\]

\[
\frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{\partial u(x, s)}{\partial s}ds(t-s)^{-\alpha} = \frac{\partial^2 u(x, t)}{\partial x^2}, \quad 0 < t \leq T,
\]
where $\alpha \in (0, 1)$, $\Gamma(\cdot)$ is a gamma function. We operate with the discrete analogue of Y. Lin, Diego [12] and A. Murio [13] to approximate the Caputo fractional derivative of order $\alpha$ with respect to time on a uniform time grid with a step of $\tau = T/K$

$$\frac{\partial^\alpha u(x, t)}{\partial t^\alpha} = \sigma_{\tau \alpha} \sum_{j=0}^{n} s_j(u^n_{i+j} - u^n_{i-j})$$  \hspace{1cm} (4)

where

$$s_j = j^{1-\alpha} - (j - 1)^{1-\alpha}, \quad \sigma_{\tau \alpha} = \frac{1}{\Gamma(2-\alpha)\tau^\alpha}.$$ \hspace{1cm} (5)

3. Finite-difference analogue of the direct problem

We substitute the derived expression into equation (1), and approximate the second derivative with respect to spatial variable with the second order in $h$. As a result, we obtain a system of linear algebraic equations with a three-diagonal matrix on the upper time layer:

$$\begin{cases}
    u^0_i = \varphi_i, & i = 1, 2, \ldots, n, \\
    u^0_k = 0, & \\
    h^2 \sigma_{\tau \alpha} \sum_{j=1}^{k} s_j (u^k_{i+j} - u^k_{i-j}) = u^k_{i-1} - 2u^k_i + u^k_{i+1}, \\
    i = 1, 2, \ldots, n-1; & u^k_n = 0, & k = 1, 2, \ldots, K.
\end{cases}$$  \hspace{1cm} (6)

Thus, it is required to solve a system of linear equations (6) with a tridiagonal matrix on each time layer, where the entire calculation background up to the lower time layer inclusive is used on the right side.

4. Numerical solution of model direct problems

We carry out a numerical verification of the difference scheme accuracy (6) on two model problems with different initial conditions and different order values of fractional derivative with respect to time $\alpha$. Then we shall compare the obtained calculation results with the exact solution obtained by the Mittag–Leffler method.

**Example 1.** We consider a direct problem with a smooth initial condition:

$$\varphi(x) = e^{-(x-l/2)^2}, \quad x \in [0, l].$$

![Figure 1](example1.png)

Figure 1. Example 1. Initial condition (left), Mittag-Leffler exact solutions and numerical solutions corresponding to $\alpha$ values (in the middle); difference scheme error at $t = T$ depending on $\alpha$ (on the right)
Calculations will be carried out at \( n = 50; \ K = 50; \ T = 1. \); \( l = 1. \) We set five values for fractional derivative \( \alpha = 0.1; \ 0.3; \ 0.5; \ 0.7; \ 0.9. \) The corresponding graphs \( u(x, T) \) and exact Mittag-Leffler solution presented in Fig. 1 have practically coincided. Fig. 1 (on the left) shows a graph of initial condition. In the middle there are exact solutions made through the finite sum of trigonometric series using the Mittag-Leffler function and numerical solutions (almost coincided). On the right there are graphs showing difference between the exact solution and a solution of the difference scheme at the final moment of time \( t = T \) for different values of the parameter \( \alpha. \) They show that the maximum error in definition of the final solution does not exceed 1%.

**Example 2.** The initial condition is set in the form of a discontinuous function:

\[
\varphi(x) = \begin{cases} 
1, & \text{for } x \geq 0.3l \text{ and } x \leq 0.7l, \\
0, & \text{otherwise}.
\end{cases}
\]

Calculations were carried out at: \( n = 50; \ K = 50; \ T = 1. \); \( l = 1. \) Same values of the fractional derivative are set \( \alpha = 0.1; \ 0.3; \ 0.5; \ 0.7; \ 0.9. \) The corresponding graphs at the initial moment of time \( u(x, 0) \) (left), the exact Mittag-Leffler solution and the numerical solutions (almost coincided) are presented in Fig. 2 (in the middle). On the right the error graphs (showing the difference between the exact solution and the one calculated by the difference scheme) have also practically coincided. An accuracy of the numerical method turned out to be slightly higher than in Example 1, though the initial condition in this example has been specified as a discontinuous function.

5. **Finite-difference analogue of the inverse problem**

Now we proceed to construction of a discrete analogue of the inverse problem, which includes a solution of the initial-boundary value problem for parabolic equation with fractional time derivative and a definition of the derivative order. Just like in a direct problem, we need to solve a system of linear algebraic equations:

\[
\begin{align*}
&u_i^K = \varphi_i, \quad i = 0, 1, 2, \ldots, n, \\
u_0^k = 0, \quad h^{2\tau} \sum_{j=1}^{k} s_j (u_i^{k-j+1} - u_i^{k-j}) = u_i^{k-1} - 2u_i^k + u_i^{k-1}, \\
i = 1, 2, \ldots, n-1; \quad u_n^k = 0, \quad k = 1, 2, \ldots, K.
\end{align*}
\]
In the inverse problem under consideration it is required to identify the order $\alpha$ of the fractional time derivative. So, we determine it from the discrete analog of the additional condition:

$$u_{n*}^K = d. \quad (8)$$

Here the spatial grid should be constructed in such a way that the observation point $\xi$ falls into the grid node with number $n_*$, in other words $\xi = n_* h$, where $n_*$ – is a natural number such that $0 < n_* < n$. Therefore, we need to find a solution to the nonlinear problem consisting of equations (7)–(8). It is nonlinear for the reason that in the system of linear equations (7) the parameter $\alpha$ – an order of the fractional time derivative must satisfy equation (8). Thus, $\alpha$ the indicator to be determined is implicitly included in equation (8), and is observed in coefficients of equation systems (7).

6. Fractional derivative order: a definition algorithm
For numerical solution of the inverse problem on definition $\alpha$ of the fractional time derivative, we construct an iterative method that uses a finite-difference analogue of the direct problem (6) at each iteration. We operate with classical iterative secant method for nonlinear equations:

1. Specifying an initial approximation of the desired parameter $\alpha_0$ we set $m = 0$ – that is an iteration number.
2. We increase the iteration number: $m = m + 1$.
3. We solve the direct problem with the given value of the order of the fractional time derivative

$$\begin{cases} u^0_i = \varphi_i, & i = 0, 1, ..., n, \\ u^0_0 = 0, & h^2 \tau \alpha^{-1}_{m-1} \sum_{j=1}^{k} s_j (u^{k-j+1}_i - u^{k-j}_i) = u^{k-1}_i - 2u^k_i + u^{k-1}_i, \\ i = 1, 2, ..., n - 1; & u^k_n = 0, \quad k = 1, 2, ..., K. \end{cases}$$

4. If $m = 1$, then we set $\alpha_1$, $\phi_1 = d$ and return to point 2. Otherwise, we assign $\phi_2 = \phi_1$, $\phi = u_{n*}^K$.
5. We determine the next approximation $\alpha_{m+1}$ by the formula:

$$\alpha_{m+1} = \alpha_m - \frac{d - \alpha_1 \phi_1}{\phi_1 - \phi_2} (\alpha_m - \alpha_{m-1}).$$

6. When the condition $|\alpha_{m+1} - \alpha_m| < \varepsilon$ is met, then we exit the iteration loop. Otherwise we return to point 2.

7. Numerical experiment
We carry out a numerical implementation of computational algorithms on the same two model problems with different initial conditions and different values of the time fractional derivative value. Then we will compare the obtained calculation results with the exact solution through the finite sum of trigonometric series using the Mittag – Leffler function.

Example 3. We consider the inverse problem with a smooth initial condition from Example 1. Calculations were carried out on the same area, grid and $\xi = l/2$.

Figure 3 shows calculation results obtained through the proposed iterative method that is used for inverse problem solution in determining the $\alpha$ order of fractional derivative for a parabolic equation. On the left we can see errors(the difference between the exact Mittag-Leffler solution with the sought $\alpha$ and the solution calculated by the proposed iterative method with the found
Figure 3. An error of numerical solutions at the final moment in time for different $\alpha$. (on the left). A graph of $\alpha$ definition depending on iteration number (on the right).

Since the additional condition is taken from the exact solution of the model example, in the middle of the region one can observe an error reduction for numerical method compared to the direct problem. The graphs on the right show an extremely fast convergence of the iterative process.

**Example 4.** We consider an inverse problem with discontinuous initial condition from Example 2. Calculations were performed on the same region, grid and $\xi = l/2$.

Figure 4. On the left there is an error of numerical solutions at the final moment of time, depending on $\alpha$. On the right there is a graph for $\alpha$ determination depending on iteration number.

At the left of Fig. 4 there is an error graph (the difference between the exact Mittag-Leffler solution with the desired $\alpha$ and the solution made by the proposed iterative method with $\alpha$ found). Since the initial condition is a discontinuous function, one can observe an error increase at points of initial condition discontinuity. Besides, since the additional condition is taken from the exact solution of the model example, one can observe a significant error reduction of the numerical method in the middle of the region. The values of the fractional derivative exponent are shown on the left, depending on the iteration number. Iterations converge quickly as well. The presented results of the computational implementation show that the suggested iterative method for identification of the fractional time derivative exponent for parabolic equation is
efficient and has the right to exist. The nature of errors is expected to jump at the points where the function breaks. At adjustment while defining, it is necessary to take into account a scheme response on a problem definition domain and an adequacy of value setting \( u(\xi, T, \alpha) = d_0 \) which was taken from the exact solution of the direct problem. The table shows the identified values for the fractional derivative exponent \( \alpha \) with respect to time for corresponding initial conditions.

| \( \alpha \)   | \( \varphi_1(x) \) | \( \varphi_2(x) \) |
|-------------|-----------------|-----------------|
| 0.1         | 0.102258        | 0.101818        |
| 0.3         | 0.303338        | 0.303081        |
| 0.5         | 0.503428        | 0.503296        |
| 0.7         | 0.702869        | 0.702825        |
| 0.9         | 0.901676        | 0.901689        |

8. Conclusion
The article presents the iterative solution method for \( \alpha \) identification of the fractional derivative order with respect to time in differential diffusion equation. The author presents the results of numerical implementation of the proposed iterative method on model examples with exact solutions in the diffusion equation for different initial conditions. The calculations showed a rather high efficiency of the proposed iterative method.

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