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DETERMINATION OF AN UNKNOWN SOURCE TERM IN A SPACE-TIME FRACTIONAL DIFFUSION EQUATION

S. TATAR, R. TINAZTEPE, S. ULUSOY

Abstract. Fractional(nonlocal) diffusion equations replace the integer-order derivatives in space and time by their fractional-order analogues and they are used to model anomalous diffusion, especially in physics. This paper deals with a nonlocal inverse source problem for a one dimensional space-time fractional diffusion equation $\partial_t^\beta u = -r^\beta(-\Delta)^{\alpha/2}u(t,x) + f(x)h(t,x)$ where $(t,x) \in \Omega_T := (0,T) \times \Omega$ and $\Omega = (-1,1)$. For the numerical solution of the inverse problem, a numerical method based on discretization of the minimization problem, steepest descent method and least squares approach is proposed. Numerical examples illustrate applicability and high accuracy of the proposed method.

1. Introduction

In this paper, we consider an inverse source problem for the following space-time fractional equation

$$\begin{cases} \dfrac{\partial^\beta}{\partial t^\beta}u(t,x) = -r^\beta(-\Delta)^{\alpha/2}u(t,x) + f(x)h(t,x), (t,x) \in \Omega_T, \\ u(t,-1) = u(t,1) = 0, \ 0 < t < T, \\ u(0,x) = 0, x \in \Omega, \end{cases} \tag{1}$$

where $\Omega_T := (0,T) \times \Omega$, $\Omega = (-1,1)$, $r > 0$ is a parameter, $f(x) \in L_2(\Omega)$, $h(t,x) \in C^1([0,T]; L^\infty(\Omega))$ are given functions, $\beta \in (0,1)$, $\alpha \in (1,2)$ are fractional order of the time and the space derivatives respectively and $T > 0$ is a final time.

The fractional-time derivative considered here is the Caputo fractional derivative of order $0 < \beta < 1$ and is defined by

$$\frac{\partial^\beta f(t)}{\partial t^\beta} := \frac{1}{\Gamma(1-\beta)} \int_0^t \frac{\partial f(r)}{\partial r} \frac{dr}{(t-r)^\beta}, \tag{2}$$

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where Γ is the Gamma function. This was intended to properly handle initial values [1, 2, 3], since its Laplace transform(LT) $s^\beta \tilde{f}(s) - s^{\beta-1} f(0)$ incorporates the initial value in the same way as the first derivative. Here, $\tilde{f}(s)$ is the usual Laplace transform. It is well-known that the Caputo derivative has a continuous spectrum [2], with eigenfunctions given in terms of the Mittag-Leffler function

$$E_\beta(z) := \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(1+\beta k)}.$$

In fact, it is easy to see that, $f(t) = E_\beta(-\lambda t^\beta)$ solves the eigenvalue problem

$$\frac{\partial^\beta f(t)}{\partial t^\beta} = -\lambda f(t), f(0) = 1,$$

for any $\lambda > 0$. This is easily verified by differentiating term-by-term and using the fact that t^p has Caputo derivative $t^{p-\beta} \frac{\Gamma(p+1)}{\Gamma(p+1-\beta)}$ for $p > 0$ and $0 < \beta \leq 1$. $0 < \beta < 1$ is taken for slow diffusion, and is related to the parameter specifying the large-time behavior of the waiting-time distribution function, see [7] and some of the references cited therein.

For $0 < \alpha < 2$, $(-\Delta)^{\alpha/2} u$ denotes the fractional Laplacian of u. It turns out that it is easier to define it by using the spectral decomposition of the Laplace operator: We take $\{\bar{\lambda}_k, \psi_k\}$ the eigenvalues and corresponding eigenvectors of the Laplacian operator in Ω with Dirichlet boundary conditions on $\partial\Omega$:

$$\begin{cases} -\Delta\psi_k = \bar{\lambda}_k \psi_k, & \text{in} \quad \Omega, \\ \psi_k = 0, & \text{on} \quad \partial\Omega. \end{cases}$$

We then define the operator $(-\Delta)^{\alpha/2}$ by

$$(-\Delta)^{\alpha/2} u := \sum_{k=0}^{\infty} c_k \psi_k(x) \mapsto -\sum_{k=0}^{\infty} c_k \bar{\lambda}_k^{\alpha/2} \psi_k(x),$$

which maps $H_0^\alpha(\Omega)$ onto $L^2(\Omega)$, where H_0^α is the fractional Sobolev space defined by

$$H_0^\alpha(\Omega) := \left\{ u = \sum_{n=1}^{\infty} a_n \psi_n : \|u\|_{H_0^\alpha}^2 = \sum_{n=1}^{\infty} a_n^2 \bar{\lambda}_n^\alpha < +\infty \right\}, \tag{3}$$

with the following equivalence

$$\|u\|_{H_0^\alpha(\Omega)} = \|(-\Delta)^{\frac{\alpha}{2}} u\|_{L_2(\Omega)}. \tag{4}$$

If f is C^1-function on $[0,\infty)$ satisfying $|f'(t)| \leq C t^{\gamma-1}$ for some $\gamma > 0$, then by (2), the Caputo derivative $\frac{\partial^\beta f(t)}{\partial t^\beta}$ of f exists for all $t > 0$ and the derivative is continuous in $t > 0$. Kilbas et al [4] and Podlubny [7] can be referred for further properties of the Caputo derivative.

In (1) the term $f(x)h(t,x)$ models a source term, and it is important to determine $f(x)$ for realizing observation data. That is to say our main goal in this paper is: Let $r > 0$ be fixed. Determine $u(t,x) = u(r,f)(t,x)$ and $f(x)$ for $t \in (0,T)$ and $x \in \Omega$ satisfying (1) and

$$u(T,x) = \varphi(x), \quad x \in \bar{\Omega}. \tag{5}$$

In this paper, we develop a numerical algorithm to solve the inverse source problem. The algorithm is based on the optimization of an error functional between the output data and the additional data. The algorithm attempts to minimize the error functional by using polynomials of a predetermined degree n. In doing so, it is assumed that the error functional is differentiable with respect to the coefficients of the polynomial which enables us to use the gradient descent method. The numerical experiments show that the algorithm is effective in practical use. A detailed analysis of the factors affecting the algorithm is also given.

The remainder of this paper comprises of four sections: In the next section, some theoretical background is recalled for the inverse source problem including the existence and uniqueness of the solution. Our numerical method is given in section 3. Some numerical examples are presented to show the efficiency of the method in section 4. In section 5, analysis of the results are given.

2. Well-Posedness of the inverse source problem

The theoretical aspect of the inverse source problem is studied in [8]. In this study, the authors have proved that the inverse problem is well-posed in the sense of Hadamard except for a discrete set of values of diffusion constants. In this section, for the sake of the reader we provide some relevant results from [8].

The formal solution to the direct problem (1) is given in the form (see [6] for details)

$$u(t,x) = \sum_{n=1}^{\infty} \bigg(\int_0^t \tau^{\beta-1} E_{\beta,\beta}\big(- \lambda_n r^\beta \tau^\beta \big) \Big\langle f(x)h(t-\tau,x), \psi_n(x) \Big\rangle d\tau \bigg) \psi_n(x), \quad (6)$$

where $\lambda_n = \big(\bar{\lambda}_n\big)^{\alpha/2}$, $\bar{\lambda}_n$ and $\{\psi_n\}_{n\geq 1}$ are eigenvalues and eigenvectors of the classical Laplace operator $-\Delta$ respectively, i.e, $-\Delta\psi_n = \bar{\lambda}_n \psi_n$. A simple calculation yields $\bar{\lambda}_n = \frac{n^2\pi^2}{4}$ hence $\lambda_n = (\frac{n\pi}{2})^\alpha$ with $\psi_n(x) = \sin\big(\frac{n\pi x}{2}\big)$ when n is even and $\psi_n(x) = \cos\big(\frac{n\pi x}{2}\big)$ when n is odd. $\big\langle \cdot\ ,\cdot \big\rangle$ denotes the standard inner product on $L_2(\Omega)$ and $E_{\alpha,\beta}(z)$ is the generalized Mittag-Leffler function defined as follows

$$E_{\alpha,\beta}(z) := \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + \beta)}, z \in \mathbb{C},$$

where $\alpha > 0$ and $\beta \in \mathbb{R}$ are arbitrary constants. We note that $\{\bar{\lambda}_n\}_{n\geq 1}$ is a sequence of positive numbers $0 < \bar{\lambda}_1 \leq \bar{\lambda}_2 \leq \cdots$, $\{\psi_n\}_{n\geq 1}$ is an orthonormal basis for $L_2(\Omega)$. It is proved in [6] that (6) is the generalized solution to the problem (1) that can be interpreted as the solution in the classical sense under certain additional conditions. We note that if one uses the substitution $\tau^\star = t - \tau$ (later replace $\tau^\star$ by τ) in (6), we get the following useful formula for the solution of (1)

$$\begin{aligned} u(t,x) = \sum_{n=1}^{\infty} \bigg(\int_0^t & (t-\tau)^{\beta-1} E_{\beta,\beta}\big(- \lambda_n r^\beta (t-\tau)^\beta \big) \\ & \times \Big\langle f(x)h(\tau,x), \psi_n(x) \Big\rangle d\tau \bigg) \psi_n(x). \end{aligned} \quad (7)$$

For the direct problem, the following theorem has been proved in [8].

Theorem 1 Let $f(x) \in L_2(\Omega)$, $h(t,x) \in C^1([0,T]; L^\infty(\Omega))$. Then there exists a unique weak solution of the problem (1) such that $u \in L_2(0,T; H_0^\alpha(\Omega))$ and

$\frac{\partial^\beta}{\partial t^\beta} u \in L_2((0,T)\times\Omega)$. Moreover, there exists a constant C such that the following inequality holds

$$\|u\|_{L_2(0,T;H_0^\alpha(\Omega))} + \|\partial_t^\beta u\|_{L_2((0,T)\times\Omega)} \leq C\|f\|_{L_2(\Omega)}. \tag{8}$$

Now we reformulate the inverse problem. For this purpose, we define the following operator equation

$$A_r f(x) + \Theta(x) = f(x), \tag{9}$$

where $A_r(f) : L_2(\Omega) \longrightarrow L_2(\Omega)$, $A_r(f)$ and $\Theta(x)$ defined by

$$A_r f(x) = \frac{\frac{\partial^\beta}{\partial t^\beta} u(r,f)(T,x)}{h(T,x)},\ \Theta(x) = \frac{r^\beta(-\Delta)^{\alpha/2}\varphi(x)}{h(T,x)}, \tag{10}$$

respectively. Here we denote $u = u(r,f)$ to emphasize the dependence of the solution $u(t,x)$ of (1) to both $r > 0$ and $f(x)$. The following lemma indicates the relationship between the operator equation (9) and the inverse problem (1), (5).

Lemma 1 [8] Let $I \subset (0,\infty)$ and $r \in I$ be fixed. Then the operator equation (9) has a solution (a unique solution) $f \in L_2(\Omega)$ if and only if the inverse problem (1), (5) has a solution (a unique solution) $\left\{u(r,f), f\right\} \in L_2(0,T;H_0^\alpha(\Omega)) \times L_2(\Omega)$.

Theorem 2 [8] A_r satisfies the following properties:

(i) For $r \in I$, the operator $A_r : L_2(\Omega) \to L_2(\Omega)$ is a compact operator.

(ii) $A_r f : I \to L_2(\Omega)$, defined by (10), is real analytic in $r \in I$ for arbitrarily fixed $f \in L_2(\Omega)$.

(iii) There exists a constant $0 < \mathcal{C}(r) < 1$ such that

$$||A_r f||_{L_2(\Omega)} \leq \mathcal{C}(r)||f||_{L_2(\Omega)},$$

where $R^\star < r$ and $R^\star > 0$ is a large number. Consequently, 1 is not an eigenvalue of the operator A_r for large $r > 0$.

By using the above properties of the operator A_r and Analytic Fredholm Theorem [9], the following existence and uniqueness theorem can be proved, see [8] for details. This theorem also guarantees that the inverse source problem considered here is well-posed in the sense of Hadamard.

Theorem 3 [8] There exists a finite set $S \subset I$ such that for $r \in I \setminus S$ and $\varphi \in H_0^\alpha(\Omega)$, the inverse problem (1), (5) has a unique solution. Moreover there exists a constant $C_{12} > 0$ such that

$$||f||_{L_2(\Omega)} + ||u||_{L_2(0,T;H_0^\alpha(\Omega))} + ||\partial_t^\beta u||_{L_2(0,T;L_2(\Omega))} \leq C_{12}||\varphi||_{H_0^\alpha(\Omega)}. \tag{11}$$

3. Overview of the method

In this section, a numerical method is proposed for the inverse source problem (1), (5). The essence of the method is to approximate the source term $f(x)$ by polynomials. Since $f(x) \in L_2(\Omega)$, there exists a sequence of polynomials converging to $f(x)$. However, finding such a sequence which guarantees the solution of the inverse problem is difficult. Our starting point is that the correct $f(x)$ will yield the solution satisfying the condition (5), hence $f(x)$ will minimize the following functional:

$$F(c) = \|u(c,T,x) - g(x)\|_2^2, \tag{12}$$

where $u(c,t,x)$ is the solution of the direct problem (1), in which $f(x)$ is replaced by the term $c(x) = c_0 + c_1 x + \cdots + c_n x^n$. Hence, the solution strategy is to approximate $f(x)$ by a polynomial of degree n that minimizes $F(c)$ for the desired n. We associate $c(x)$ to the vector $c = (c_0, \cdots, c_n)$, hence $F(c)$ is a real valued function of n variables.

The method for minimizing $F(c)$ depends on the properties of $u(c,T,x)$. In our case, the convexity or differentiability of $F(c)$ is not clear due to the term $u(c,x,t)$. However, we do not envision a major drawback in assuming the differentiability of $F(c)$ in numerical implementations. For this reason, we proceed the minimization of $F(c)$ by the steepest descent method which will utilize the gradient of F.

In this method, the algorithm starts with an initial point b_0, then the point providing the minimum is approximated by the points

$$b_{i+1} = b_i + \triangle b_i,$$

where $\triangle b_i$ is the feasible direction which minimizes

$$E(\triangle b) = F(b_i + \triangle b).$$

This procedure is repeated until a stop criterion is satisfied, i.e, $\|\triangle b_i\| < \epsilon$ or $|F(b_{i+1}) - F(b_i)| < \epsilon$ or a certain number of iterations. In the minimization of $E(\triangle b)$, we use the following estimate on $u(b_i + \triangle b, T, x)$

$$u(b_i + \triangle b, T, x) \simeq u(b_i, T, x) + \nabla u(b_i, T, x) \cdot \triangle b,$$

where ∇denotes the gradient of $u(b,T,x)$ with respect to b. Hence $E(\triangle b)$ turns out to be

$$E(\triangle b) = \|\nabla u(b_i, T, x) \cdot \triangle b + u(b_i, T, x) - g(x)\|_2^2.$$

In numerical calculations, we note that $\|\cdot\|_2$ can be discretized by using a finite number of points in $[-1,1]$, i.e., for $x_1 = 0 < x_2 < \cdots < x_q = 1$, hence $E(\triangle b)$ has its new form as

$$E(\triangle b) \simeq \sum_{k=1}^{q} (u(b_i, T, x_k) + \nabla u(b_i, T, x_k) \cdot \triangle b - g(x_k))^2. \tag{13}$$

Now the minimization of this problem is a least squares problem whose solution leads to the following normal equation (see [5])

$$AA^T \triangle b = A^T K,$$

where

$$A = \left[\nabla u(b_i, T, x_1)^T \cdots \nabla u(b_i, T, x_q)^T\right],$$

and

$$K = [u(b_i, T, x_1) - g(x_1) \cdots u(b_i, T, x_q) - g(x_q)]^T.$$

Now the optimal direction is found by

$$\triangle b = (A^T A)^{-1} A^T K. \tag{14}$$

In forming A, the computation (or estimation) of s^{th} component of the vector $\nabla u(b_i, T, x_k)$ can be obtained by

$$\frac{u(b_i + he_s, T, x_k) - u(b_i, T, x_k)}{h}, \tag{15}$$

where e_s is the standard unit vector whose s^{th} component is 1 and h is the differential step.

Our algorithm consists of the following steps:

Step 1. Set b_0, n and a stop criterion k or ϵ (iteration number or size of $\triangle b_i$).

Step 2. Calculate $\triangle b_i$ using 14 and set $b_{i+1} = b_i + \triangle b_i$.

Step 3. Stop when the stop criterion is achieved.

4. Numerical examples

In this section we examine the algorithm with two inverse problems. In implementing the algorithm, finding $u(c, T, x)$ is a crucial step and its precision directly affects the efficiency of the algorithm. In finding $u(c, T, x)$, the formula (7) is used.

In our examples, the correct $f(x)$ is predetermined and the corresponding $g(x)$ is obtained from the numerical solution of the direct problem where $r, T = 1$ and $h(t, x)$, α, β are predetermined. The expected solution is the nth degree Taylor polynomial approximation of $f(x)$ for the given n. The computations have been carried out in MATLAB.

Due to the discretization of the problem, many variables emerge in computations. These variables and their values in our computations are listed below:

(1) The dimension of c in $F(c)$ to approximate $f(x)$: $n = 2, 3, 4, 5, 6$ and 7 are taken in the examples.
(2) Initial guess for c: All initial guesses for the coefficients are taken to be vectors composed of 1's in order to get an objective observation.
(3) Differential step h in (15): $h = 0.1$ are taken on the examples.
(4) Number of the points taken on $[-1, 1]$, i.e., q in (13): $q = 20$ and $q = 40$ are taken in the first example and the second example respectively.
(5) Sensitivity of $E_{\beta,\beta}$: is taken to be 10^{-6}.
(6) Upper bound for summing index in $u(c, t, x)$: is taken to be 20 and 40 for the first and second example respectively.
(7) Stop criterion: $\|\triangle b_i\| < \epsilon$ or maximum iteration number M with $\epsilon = 0.01$ and $M = 100$.

Example 1. $\alpha = 1.5$, $\beta = 0.5$, $h(t, x) = 1$, $f(x) = \sin x$. The expected solutions are the Taylor polynomials for $\sin x$. See Table 1.

Example 2. $\alpha = 1.5$, $\beta = 0.5$, $h(t, x) = t$, $f(x) = e^{-x}$. The expected solutions are the Taylor polynomials for e^{-x}. See Table 2.

TABLE 1. Initial guesses for $n = 2, 3$,4,5,6 and 7

Initial guesses	Coefficients of the Taylor Polynomials of the solution
(1,1)	(0.0000 1.0972)
(1,1,1)	(-0.0000 1.0972 0.0002)
(1,1,1,1)	(-0.0000 0.9579 0.0002 0.3518)
(1,1,1,1,1)	(0.0001 0.9579 -0.0011 0.3519 0.0018)
(1,1,1,1,1,1)	(0.0001 0.9901 -0.0010 0.1395 0.0016 0.2488)
(1,1,1,1,1,1,1)	(-0.0 0.9901 -0.0002 0.1393 0.0034 0.2490 -0.0048)

TABLE 2. Initial guesses for $n = 2, 3$,4,5 and 6

Initial guesses	Coefficients of the Taylor Polynomials of the solution
(1,1)	(0.9874, -1.1858)
(1,1,1)	(0.7355 -1.1858 1.4319)
(1,1,1,1)	(0.7355 -0.7727 1.4320 -1.0864)
(1,1,1,1,1)	(0.7744 -0.7727 0.7757 -1.0864 1.0964)
(1,1,1,1,1,1)	(0.7744 -0.8633 0.7758 -0.4587 1.0963 -0.7605)
(1,1,1,1,1,1,1)	(0.7683 -0.8632 0.9705 -0.4588 0.2912 -0.7605 0.7618)

5. Analysis of Results

The experimental results provide coarse approximations of the functions sought and are satisfactory to some extent, especially with the given initial guesses. Since the analytical solution $u(c, t, x)$ includes infinite sum, integration for each t and the inner product in L_2 which is also an integration over the real line, the computational errors contribute much to the results. In finding the solution of the direct problem $u(c, t, x)$, the upper bound for the summing index seems to be the most important among the other computational factors. The experiments show that using a higher summing index does not enhance the result. This is due to the rising of total error because of the errors coming from each summand.

In addition to the complexity of the analytical form of the solution of the direct problem, the error functional is not known to satisfy some properties which guarantees the convergence of the algorithm. Since the error functional $F(c)$ given by 12 is not convex, it is most likely that there are many local minimizers of the error functional which requires the initial guesses to be close enough to the Taylor coefficients of the correct solution in a given dimension. This makes the problem ill-posed to some extent. In the experiments, the initial guesses are taken to be relatively far from the Taylor coefficients of the functions sought and same initial guesses are tested to get an objective result. Related to this issue, one other important point is the dimension of c. It seems that using higher dimensions of c enhances the results to some extent however the computation time severely increases.

Another fact about the algorithm is that the implementation of the algorithm requires the differentiability of the error functional with respect to c. This is assumed in deriving the algorithm but it is not theoretically clear as pointed in the previous section. In the implementation, the differential step is taken to be $h = 0.1$, however the results with $h = 0.01$, not presented above, does not show a significant difference.

As a result the high computational complexity of the form of the analytical solution of the direct problem, the lack of some properties such as convexity and/or differentiability of the error functional and using only polynomial approximations in error functional are the main setbacks of the algorithm. Hence, the coarseness of these results is expected. The properties of the error functional for certain properties of $h(t, x)$ should be investigated and finding a more computational friendly form of the solution of the direct problem will contribute much to the numerical solutions of the inverse problem.

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Department of Mathematics, Faculty of Education, Zirve University, Sahinbey, Gaziantep,, 27260, Turkey

E-mail address: salih.tatar@zirve.edu.tr

Department of Mathematics, Faculty of Education, Zirve University, Sahinbey, Gaziantep,, 27260, Turkey

E-mail address: ramazan.tinaztepe@zirve.edu.tr

Department of Mathematics, Faculty of Education, Zirve University, Sahinbey, Gaziantep,, 27260, Turkey

E-mail address: suleyman.ulusoy@zirve.edu.tr