Generalized time fractional IHCP with Caputo fractional derivatives

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Abstract. The numerical solution of the generalized time fractional inverse heat conduction problem (GTFIHCP) on a finite slab is investigated in the presence of measured (noisy) data when the time fractional derivative is interpreted in the sense of Caputo. The GTFIHCP involves the simultaneous identification of the heat flux and temperature transient functions at one of the boundaries of the finite slab together with the initial condition of the original direct problem from noisy Cauchy data at a discrete set of points on the opposite (active) boundary. A finite difference space marching scheme with adaptive regularization, using trigonometric mollification techniques and generalized cross validation is introduced. Error estimates for the numerical solution of the mollified problem and numerical examples are provided.

1. Introduction
Fractional derivatives and partial fractional derivatives have been applied recently to the numerical solution of problems in fluid and continuum mechanics \cite{1}, viscoelastic and viscoplastic flow \cite{2} and anomalous diffusion (superdiffusion, non-Gaussian diffusion, subdiffusion) \cite{3, 4, 5, 6}. Numerous citations to several other applications of fractional derivatives to problems in physics, finance and hydrology can also be found in these articles.

Time fractional diffusion equations (TFDE) arise by replacing the standard time partial derivative in diffusion equations with a time fractional partial derivative, attempting to generalize the classical Fick (or Fourier) law to describe phenomena with long memory where the rate of diffusion might be inconsistent with the classical Brownian motion model.

The main purpose of this paper is to introduce and analyze a stable space marching numerical method for the approximate solution of a generalized time fractional inverse heat conduction problem (GTFIHCP) when the time fractional derivative in the governing partial differential equation is formulated with Caputo fractional derivatives. The GTFIHCP involves the simultaneous identification of the heat flux and temperature transient functions at one of the boundaries of the finite slab together with the initial condition of the original direct problem from noisy Cauchy data at a discrete set of points on the opposite (active) boundary. As such, this investigation can be interpreted as an important extension of the work presented in \cite{7}, where the classical time fractional inverse heat conduction problem (TFIHCP) is solved under the assumption that the initial condition for the direct problem is known.

Previous background work on simultaneous identification of parameters in parabolic equations, systems of parabolic equations, inverse heat conduction problems and generalized inverse heat conduction problems in 1 and 2 space dimensions can be found in \cite{8, 9, 10, 11, 12}.
The manuscript is organized as follows: in section 2 we give a rendition of Caputo fractional derivatives as an ill-posed problem when the data is not known exactly and regularization is required. We briefly describe the trigonometric mollification technique [13], that provides a functional representation of the mollified computed approximations of Caputo fractional derivatives and guarantees excellent fitting near the endpoints of the intervals and the usage of small values of the regularization parameters –radii of mollification- if necessary. In section 3, we concentrate our attention on time fractional diffusion equations and in section 4 we include typical numerical examples.

2. Caputo Derivatives

The Caputo fractional derivative of order \(\alpha\), \(0 < \alpha \leq 1\), of a differentiable function \(g\) defined on the interval \([0,T]\), is given by

\[
(D^{(\alpha)} g)(t) = \frac{1}{\Gamma(1-\alpha)} \int_{0}^{t} \frac{g'(s)}{(t-s)^\alpha} \, ds, \quad 0 \leq t \leq T, \quad 0 < \alpha < 1, \tag{1}
\]

\[
(D^{(\alpha)} g)(t) = \frac{dg(t)}{dt}, \quad 0 \leq t \leq T, \quad \alpha = 1.
\]

For further details and a historical perspective on fractional derivatives, see [14].

2.1. Fractional Derivatives as Ill-Posed Problems

For the numerical computation of Caputo fractional derivatives when the data function \(g\) is measured with noise, we regularize the problem using mollification techniques following [15]. For a general introduction to mollification theory as well as important practical implementation details, see [16, 17].

Without loss of generality, we restrict our attention to functions defined on the interval \(I = [0,1]\).

In the presence of noisy data \(g^\epsilon(t)\), a perturbed version of the exact data function \(g(t)\), instead of recovering \(D^{(\alpha)} g\) we look for a mollified solution \(J_{\delta}(D^{(\alpha)} g^\epsilon)\) obtained from (1) by convolution with a certain Gaussian kernel \(\rho_{\delta}\), which depends on a scalar regularization parameter \(\delta\) known as the mollification radius. More precisely,

\[
J_{\delta}(D^{(\alpha)} g^\epsilon)(t) = (D^{(\alpha)} g^\epsilon * \rho_{\delta})(t) \tag{2}
\]

\[
= \frac{1}{\Gamma(1-\alpha)} \int_{0}^{t} \frac{(J_{\delta}g^\epsilon)'(s)}{(t-s)^\alpha} \, ds.
\]

The main property of the method is given below [15].

**Theorem 1** If the functions \(g'\) and \(g^\epsilon\) are uniformly Lipschitz on \(I\) and \(\|g - g^\epsilon\|_{\infty,I} \leq \epsilon\), then there exists a constant \(C\), independent of \(\delta\), such that on \(I_{\delta} = [3\delta,1-3\delta]\),

\[
\left\|J_{\delta}(D^{(\alpha)} g^\epsilon) - D^{(\alpha)} g\right\|_{\infty,I_{\delta}} \leq \frac{C}{(1-\alpha)\Gamma(1-\alpha)} \left(\delta + \frac{\epsilon}{\delta}\right).
\]

Stability is valid for each fixed \(\delta > 0\) and the optimal rate of convergence is obtained by choosing \(\delta = O(\sqrt{\epsilon})\).

The mollified Caputo fractional derivative, computed from noisy data, tends uniformly to the exact solution as \(\epsilon \to 0\), \(\delta = \delta(\epsilon) \to 0\). This establishes the consistency, stability and formal convergence properties of the procedure.
2.2. **Trigonometric Mollification**

To numerically approximate \( J_δ(D^{(a)}g^ε) \), a quadrature formula for the convolution equation (2) is needed. Introducing a uniform partition \( K \) of the interval \( I = [0,1] \), with elements \( t_i = ik \), \( i = 0,1,...,n-1 \), \( (n-1)k = 1 \), the discrete noisy data function \( G^ε \) (restriction of the function \( g^ε \) to \( K \)), is replaced by \( G^ε(t_i) \) by subtracting a suitable linear trend. That is,

\[
G^ε(t_i) = G^ε(t_i) - (G^ε(1) - G^ε(0))t_i, \quad i = 0,1,...,n-1,
\]

and we observe that the modified discrete function \( G^ε \) satisfies the homogeneous boundary conditions \( G^ε(0) = G^ε(1) = 0 \). We now extend \( G^ε \) as an odd function and determine the trigonometric polynomial \( S^*_n(t) \), of period 2, interpolating \( G^ε(t_i) \) at the points \( t_i, i = 1,...,n-2 \).

Thus,

\[
S^*_n(t) = \sum_{k=1}^{n-2} b_k \sin(k\pi t)
\]

where the coefficients \( b_k \) are the unique solution of the least square problem associated with the orthogonal functions \( \varphi_k = \{ \sin(k\pi t_i),\ldots,\sin(k\pi t_{n-2}) \}, k = 1,2,...,n-2 \), in the unit interval.

Once the radius of mollification is automatically selected (see \[17\]), the mollified trigonometric interpolant is given by the simple formula

\[
(J_δS^*_n)(t) = (S^*_n * ρ_δ)(t)
\]

\[= \sum_{k=1}^{n-2} e^{-\frac{1}{4}k^2\pi^2\delta^2} b_k \sin(k\pi t),\]

and the approximation to (2), denoted \((D^{(a)}S^*_n)_δ\), becomes

\[
(D^{(a)}S^*_n)_δ(t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{(J_δS^*_n)'(s) + G^ε(0) - G^ε(1)}{(t-s)^\alpha} ds.
\]

At the grid points, formula (4) can be written as

\[
(D^{(a)}S^*_n)_δ(t_i) = \frac{1}{\Gamma(1-\alpha)} \sum_{j=0}^{i} \int_{j\delta}^{(j+1)\delta} \frac{(J_δS^*_n)'(s) + G^ε(0) - G^ε(1)}{(t_i-s)^\alpha} ds
\]

\[= \frac{1}{\Gamma(1-\alpha)} \sum_{j=0}^{i} \int_{j\delta}^{(j+1)\delta} \frac{(J_δS^*_n)'(s) + G^ε(0) - G^ε(1)}{(t_i-s)^\alpha} ds,
\]

and on each element of the partition the corresponding integral is approximated by a Gaussian quadrature of two points, except for the first five intervals where an adaptive Gaussian quadrature is implemented. (See \[13\] for computational details.) The discrete computed approximations of (2) are denoted \((D^{(a)}G^ε)_δ(t_i), i = 1,...,n-1 \) and satisfy the following estimates \[15\].

**Theorem 2**  If the functions \( g^ε \) and \( g^ε \) are uniformly Lipschitz on \( I \) and \( G \) and \( G^ε \), the discrete versions of \( g \) and \( g^ε \) respectively, satisfy \( \| G - G^ε \|_{\infty,K} \leq \epsilon \), then

\[
\left\| J_δ(D^{(a)}g^ε) - (D^{(a)}G^ε)_δ \right\|_{\infty,K} \leq \frac{C \Delta t}{\Gamma(1-\alpha)(1-\alpha)}.
\]

**Corollary 3**  Under the hypothesis of Theorems 1 and 2,

\[
\left\| (D^{(a)}G^ε)_δ - (D^{(a)}g) \right\|_{\infty,K} \leq \frac{C}{\Gamma(1-\alpha)(1-\alpha)}(\delta + \frac{\epsilon}{\delta} + \Delta t).
\]
3. Generalized Time Fractional IHCP

In this section we present a straightforward generalization of the classical GIHCP [16, 17, 9], by allowing the fractional order of differentiation, \( \alpha \), to vary between 0 and 1.

We consider a one dimensional GTFIHCP on a finite slab of width \( x_0 \leq 1 \) in which the temperature \( u(x_0, t) \) and the heat flux \( u_x(x_0, t) \) at the boundary \( x = x_0 \) together with the initial temperature \( u(x, 0) = u_0(x) \) at \( t = 0 \) are desired and unknown, and the temperature \( u(0, t) \) and the heat flux \( u_x(0, t) \) at the active boundary \( x = 0 \) are approximately known. This problem has not been solved before and it is a useful contribution to the community interested in the modelling with fractional derivatives as can be seen by looking at [1, 2, 3, 4, 5, 6]. We assume a normalized (dimensionless) linear heat conduction equation with unit fractional diffusivity.

The GTFIHCP is described mathematically by the system

\[
\begin{align*}
  u_{xx}(x, t) &= D_t^{(\alpha)} u(x, t), & 0 < t < 1, & 0 < x < x_0, \\
  u(0, t) &= \eta^{(t)}, & 0 \leq t \leq 1, & \text{data}, \\
  u_x(0, t) &= \sigma^{(t)}, & 0 \leq t \leq 1, & \text{data}, \\
  u(1, t) &= \lambda^{(t)}, & 0 \leq t \leq 1, & \text{unknown}, \\
  u_x(1, t) &= \beta^{(t)}, & 0 \leq t \leq 1, & \text{unknown}, \\
  u(x, 0) &= u_0(x), & 0 \leq x \leq 1, & \text{unknown},
\end{align*}
\]

where \( \eta \) and \( \sigma \) are not known exactly. The available data functions, \( \eta^{(t)} \) and \( \sigma^{(t)} \), are measured approximations of \( \eta \) and \( \sigma \) respectively and they satisfy the error estimates \( \| \eta - \eta^{(t)} \|_{\infty, I} \leq \epsilon_1 \) and \( \| \sigma - \sigma^{(t)} \|_{\infty, J} \leq \epsilon_2 \).

Our main objective is to describe the numerical procedure for the simultaneous approximation of the unknowns in (5). For that matter, we work with a maximum level of noise in the data given by \( \epsilon = \max \{ \epsilon_1, \epsilon_2 \} \). Since the GTFIHCP is extremely ill-posed in the high frequency components [18], it must be regularized. This is accomplished by mollifying system (5). In the stabilized (mollified) problem, \( v = J_\delta u \) and \( v_x = J_\delta u_x \) satisfy

\[
\begin{align*}
  v_{xx} &= D_t^{(\alpha)} v, & 0 < t < 1, & 0 < x < x_0, \\
  v(0, t) &= J_\delta \eta^{(t)}, & 0 \leq t \leq 1, \\
  v_x(0, t) &= J_\delta \sigma^{(t)}, & 0 \leq t \leq 1, \\
  v(1, t) &= J_\delta \lambda^{(t)}, & 0 \leq t \leq 1, & \text{unknown}, \\
  v_x(1, t) &= J_\delta \beta^{(t)}, & 0 \leq t \leq 1, & \text{unknown}, \\
  v(x, 0) &= v_0(x), & 0 \leq x \leq x_0, & \text{unknown}.
\end{align*}
\]

Now we introduce the numerical method for the solution of system (6) on the \([0, x_0] \times [0, 1]\) region of the \((x, t)\) plane. It is a combination of a stable space marching finite difference scheme with trigonometric \( \delta \)-mollification at each step, making the actual filtering procedure adaptive.

For some positive integers \( M \) and \( N \), let \( h = \frac{x_0}{M} \) and \( k = \frac{1}{N} \) be the parameters of the finite difference discretization. We denote by \( R^n_j \), \( W^n_j \), and \( Q^n_j \) the computed approximations of the mollified temperature \( v(jh, nk) \), mollified heat flux \( v_x(jh, nk) \), and time fractional partial derivative of mollified temperature \( D_t^{(\alpha)} v(jh, nk) \), respectively. The system to be solved is

\[
\begin{align*}
  R^n_{j+1} &= R^n_j + h W^n_j, \\
  W^n_{j+1} &= W^n_j + h Q^n_j.
\end{align*}
\]

The main difference with the corresponding system in [9, 17] is the approximation of the Caputo fractional derivatives which near \( t = 0 \) have to be computed with great care because those values depend on the limiting behavior and they have to be consistent with the initial condition of the original time fractional differential equation.
For error estimates, we begin by defining the discrete error functions

\[ \Delta R^n_j = R^n_j - v(jh, nk), \]
\[ \Delta W^n_j = W^n_j - v_x(jh, nk). \]

Next, we introduce the notation \[ |Y_j| = \max_{1 \leq n \leq N} |Y^n_j| \]
and define \( \delta > 0 \) to be the smallest mollification parameter required in the computations. Finally, setting \( \Delta_j = \max\{|\Delta R_j|, |\Delta W_j|\} \), we obtain the following estimates:

\[ \Delta_0 \leq \frac{C}{\delta}(\epsilon + k) \]

where \( C \) is a constant independent of \( \delta, k, h \) and \( \epsilon \) and

\[ \Delta_M \leq (\exp\left(\frac{C_\alpha}{\delta}\right)\Delta_0 + \frac{\epsilon^2}{C_\alpha} - 1)O(k + h), \]

where \( C_\alpha = \frac{1}{\Gamma(1 - \alpha)(1 - \alpha)} \).

The details related to the algorithm and the error estimates will be presented elsewhere. In the next section we verify the quality of our numerical method by considering two typical numerical examples.

4. Numerical Examples

We assume a finite slab of width \( x_0 = 1/2 \) with the number of space and time divisions to be \( M \) and \( N \) respectively, \( h = x_0/M \) and \( k = 1/N \). The maximum level of noise in the data functions is \( \epsilon \).

Discretized measured approximations of the initial data for the inverse problem at \( x = 0 \) are simulated by adding random errors to the exact data functions. Specifically, for a boundary data function \( s(t) \), its discrete noisy version is

\[ s^n_\epsilon = s(t_n) + \epsilon_n, \quad n = 0, 1, \ldots, N, \]

where the \( (\epsilon_n) \)'s are Gaussian random variables with variance \( \sigma^2 = \epsilon^2 \).

In order to generate the necessary data for modeling the GTFIHC, we need to solve the corresponding TFDE (the direct problem.) To that end, we implement the unconditionally stable implicit finite difference method introduced in [19].

The temperature and heat flux errors at the boundary \( x = 1/2 \) are measured by the weighted, relative, \( l^2 \)- norm defined by

\[ \left[ \frac{1}{M+1} \sum_{n=0}^{M} |R^n_M - u(1, nk)|^2 \right]^{1/2}, \]

where the “exact” value \( u(1, nk) \) is the computed (approximate) temperature solution of the direct problem.

**Example 1**

This prototype example emphasizes the reconstruction of an initial temperature distribution with an interior maximum together with the estimation of transient temperature and heat flux functions at \( x = 1/2 \), from transient data measured at \( x = 0 \).

We solve the direct time fractional diffusion equation imbedded in (6) with initial and boundary conditions \( u(x, 0) = x(1/2 - x), u(0, t) = \sin t, u(1/2, t) = t^2(t - 1) \), time fractional orders \( \alpha = 0.10, 0.50, 0.90 \) and grid sizes \( h = 0.01 \) and \( k = 1/256 \), respectively.
Example 1

For the direct problem we are interested in the solutions corresponding to the heat fluxes at the surfaces $x = 0$ and $x = 1/2$, obtained by numerically differentiating the computed temperature distributions up to the boundaries.

After adding noise to the data of maximum magnitude $\epsilon = 0.05$ to generate $u'(0, t)$ and $u_x'(0, t)$ at the time grid points of the active boundary $x = 0$, system (6) is then solved with parameters $h = 0.02, 0.01$ and $k = 1/64, 1/128, 1/256$. Relative errors are listed in tables 1 and 2. Some approximate reconstructions are illustrated in figures 1 and 2 for temperatures and heat fluxes at $x = 1/2$ and figure 5 for initial temperature distributions at $t = 0$, for typical parameters values $\alpha = 0.50, h = 0.01, k = 1/128$, and $\epsilon = 0.05$.

![Figure 1](image1.png)  
**Figure 1.** Temperatures at $x = 1/2$.

![Figure 2](image2.png)  
**Figure 2.** Heat fluxes at $x = 1/2$.

Example 2

As a second model, with the same parameters as in example 1, the implicit method is applied to the solution of the TFDE with a monotonically increasing initial temperature $u(x, 0) = 4x^2$ and boundary conditions $u(0, t) = 0$ and $u(1/2, t) = e^{-t}$.

The Cauchy data for the GTFIHCP in the time interval $[0, 1]$ at the boundary $x = 0$, is then utilized to solve the system (6) using the mollified space marching scheme (7) with noisy data $u'(0, t)$ and $u_x'(0, t)$ and the same parameter values as in example 1.

The results are summarized in table 3 and figures 3, 4 and 6.
Table 2. Example 1. TFIHCP $l_2$-error norms at $t = 0$ in the interval $[0, 1/2]$.

| $\epsilon = 0.05$ | Temp. $h = 1/50$ | Temp. $h = 1/100$ |
|-------------------|-------------------|-------------------|
| $k = 1/64$ | 0.0522 | 0.0465 |
| $k = 1/128$ | 0.0723 | 0.0505 |
| $k = 1/256$ | 0.0785 | 0.0651 |
| $\alpha = 0.10$ | 0.0414 | 0.0647 |
| $\alpha = 0.50$ | 0.0607 | 0.0372 |
| $\alpha = 0.90$ | 0.0581 | 0.0485 |

Figure 3. Temperatures at $x = 1/2$.

Figure 4. Heat fluxes at $x = 1/2$.

Table 3. Example 2. TFIHCP $l_2$-error norms at $x = 1/2$ in the interval $[0, 1]$.

| $\epsilon = 0.05$ | Temp. $h = 1/50$ | Heat Flux $h = 1/50$ | Temp. $h = 1/100$ | Heat Flux $h = 1/100$ |
|-------------------|------------------|---------------------|------------------|---------------------|
| $k = 1/64$ | 0.0465 | 0.0501 | 0.0505 | 0.0651 |
| $k = 1/128$ | 0.0373 | 0.0372 | 0.0307 | 0.0345 |
| $k = 1/256$ | 0.0373 | 0.0465 | 0.0501 | 0.0576 |
| $\alpha = 0.10$ | 0.0402 | 0.0510 | 0.0651 | 0.0764 |
| $\alpha = 0.50$ | 0.0742 | 0.0798 | 0.0787 | 0.0798 |
| $\alpha = 0.90$ | 0.0863 | 0.0903 | 0.0863 | 0.0863 |

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**Figure 5.** Exact and computed initial temperatures in example 1.

**Figure 6.** Exact and computed initial temperatures in example 2.

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