Stable numerical solution of a fractional-diffusion inverse heat conduction problem

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Abstract

The ill-posed problem of attempting to recover the boundary temperature and the heat flux functions from one measured transient data temperature at some interior point of a one-dimensional semi-infinite conductor when the governing linear diffusion equation is of fractional type is discussed. A simple algorithm based on space marching mollification techniques is introduced for the numerical solution of the discrete problem. Stability bounds, error estimates and numerical examples of interest are also presented.

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1. Introduction

It is shown in [1,2] that the classical diffusion equation, requiring second spatial derivatives and first time derivatives can be reduced to a simpler equation involving only a first-order spatial derivative and a half-order time derivative under the assumptions of linear unidirectional heat transport through a semi-infinite domain with common constant initial and asymptotic boundary conditions (see also [3]). The fractional partial derivative equation is then utilized to recover the heat flux at the active boundary from the knowledge of the analytic temperature function given also at the active boundary.

Some recent applications to diffusion processes involving fractional derivative formulations for direct problems (superdiffusion, non-Gaussian diffusion) can be found, for example, in [4,5] and the references therein.

In this paper we study the more general ill-posed problem of attempting to recover the temperature and the heat flux functions at the active boundary from one measurement of the transient temperature function at some arbitrary interior space location of the semi-infinite domain. Our main purpose is to present and analyze a stable method, based on marching mollification techniques, for the numerical computation of the boundary functions.

In what follows we refer to this problem as the fractional inverse heat conduction problem (FIHCP).

The half-fractional time derivative that appears in the FIHCP corresponds to the Riemann–Liouville definition.

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The Riemann–Liouville fractional derivative of order \( \alpha, 0 < \alpha < 1 \), of an integrable function \( g \) defined on the interval \([0, T]\), is given by the convolution integral

\[
(D^{(\alpha)} g)(t) = \frac{1}{\Gamma(1-\alpha)} \frac{d}{dt} \int_0^t g(s)(t-s)^{-\alpha} ds, \quad 0 \leq t \leq T, 0 < \alpha < 1,
\]

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

where \( \Gamma(.) \) is the Gamma function.

For further details on fractional derivatives and a general historical perspective, see [6].

The manuscript is organized as follows. In Section 2 the original ill-posed problem and the associated regularized (mollified) problem, respectively, are formulated and analyzed. The numerical procedure and the error analysis of the algorithm are investigated in Section 3. Numerical examples are provided in Section 4.

2. Description of the problem

We consider a one-dimensional FIHCP on a semi-infinite slab in which the temperature \( U(t) \) and the heat flux \( q(t) \) on the active boundary \( x = 0 \) are desired and unknown, and the temperature \( f(t) \) at some interior point \( x = x_1 > 0 \) is approximately measurable. We assume a normalized (dimensionless) linear heat conduction with constant diffusivity and common constant initial temperature distribution and asymptotic boundary temperature.

Following [1], the mathematical description of the FIHCP is listed next. The unknown temperature \( u(x, t) \) satisfies

\[
\frac{\partial}{\partial x} u(x, t) = -a^{-1/2} \frac{\partial}{\partial t} \frac{\partial}{\partial t} u(x, t) + u_{\infty}(\pi a t)^{-\frac{1}{2}}, \quad x > 0, t \geq 0,
\]

\[
u(x_1, t) = f(t), \quad \text{with approximate data function } f_m(t), \quad x_1 > 0, t > 0,
\]

\[
u(0, t) = U(t), \quad \text{unknown, } t \geq 0,
\]

\[-\frac{\partial}{\partial x} u(0, t) = q(t), \quad \text{unknown, } t \geq 0,
\]

where \( a \) is the constant diffusivity coefficient, \( u_{\infty} = u(x, 0) = \lim_{x \to \infty} u(x, t) = \text{const.} \), and the half-time differentiation indicates the Riemann–Liouville fractional derivative.

2.1. Ill-posedness of FIHCP

In order to simplify the Fourier analysis of the FIHCP, and in the rest of the paper, we assume without loss of generality, \( a = 1, u_{\infty} = 0 \) and all the functions extended to the whole line \(-\infty < t < \infty \) by defining them to be zero for \( t < 0 \) whenever it is necessary. We also assume that all the functions involved are \( L_2 \) in \( \mathbb{R} \) and use the corresponding \( L_2 \) norm, as defined below, to measure errors:

\[
\| y \| = \left( \int_{\mathbb{R}} |y(t)|^2 dt \right)^{1/2}.
\]

If the Fourier transform of a function \( y(t) \) is written as

\[
\hat{\mathcal{Y}}(w) = \int_{-\infty}^{\infty} y(t) e^{-iwt} dt, \quad i = \sqrt{-1},
\]

then the Fourier inversion formula reads

\[
y(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \hat{\mathcal{Y}}(w) e^{iwt} dw,
\]

and Parseval’s identity takes the form

\[
\| y \| = \sqrt{2\pi} \| \hat{y} \|.
\]
Fourier transforming (1) with respect to \( t \), we have
\[
\frac{\partial}{\partial x} \hat{u}(x, w) = -\sqrt{i}w \hat{u}(x, w), \quad 0 < x < x_1, -\infty < w < \infty,
\]
utilizing the fact, [6] page 112, that
\[
\Im \left\{ \frac{\partial}{\partial t} u(x, t), (x, w) \right\} = \sqrt{i}w \hat{u}(x, w).
\]
The first-order ordinary differential equation (4) has the general solution
\[
\hat{u}(x, w) = \hat{u}(0, w)e^{-\sqrt{i}wx},
\]
and it follows that
\[
\hat{u}(x, w) = -\frac{1}{\sqrt{i}w} \frac{\partial}{\partial x} u(0, w)e^{-\sqrt{i}wx}.
\]
Setting \( x = x_1 \) in the last two equalities we get the estimates
\[
|\hat{u}(0, w)| \leq e^{\sqrt{|w|^2}x_1}|\hat{f}(w)|
\]
and
\[
\left| -\frac{\partial}{\partial x} \hat{u}(0, w) \right| \leq \frac{|w|}{2} e^{\sqrt{|w|^2}x_1}|\hat{f}(w)|.
\]
This shows that attempting to solve for \( u(0, t) \) or \( -\frac{\partial}{\partial x} u(0, t) \) from a given \( f(t) = u(x_1, t) \), amplifies the error in the high frequency components by the factor \( \exp(\sqrt{|w|^2}x_1) \) and, consequently, the FIHCP is a severely ill-posed problem for high frequency components.

2.2. Stabilized FIHCP

In this section we use the mollification method to stabilize the FIHCP. We introduce the function
\[
\rho_\delta(t) = \frac{1}{\delta \sqrt{\pi}} \exp \left( \frac{-t^2}{\delta^2} \right),
\]
the one-dimensional Gaussian kernel of “blurring” radius \( \delta > 0 \). The kernel \( \rho_\delta \) is always positive, nearly vanishes outside the interval \((-3\delta, 3\delta)\) and \( \int_{-\infty}^{\infty} \rho_\delta(s)ds = 1 \).

The convolution of a function \( f \) with \( \rho_\delta \) is defined by
\[
J_\delta f(t) = (\rho_\delta * f)(t) = \int_{-\infty}^{\infty} \rho_\delta(t - s) f(s)ds \approx \int_{t-3\delta}^{t+3\delta} \rho_\delta(t - s) f(s)ds.
\]
For any locally integrable function \( f \), \( J_\delta f \) is infinitely differentiable and \( \| J_\delta f - f \| \to 0 \) as \( \delta \to 0 \), the convergence being uniform on any compact set where \( f \) is continuous [8]. The basic idea of the mollification method is that instead of attempting to find the point values of the boundary temperature function \( u(0, t) = U(t) \) and the heat flux function \( -\frac{\partial}{\partial x} u(0, t) = q(t) \), we attempt to reconstruct the \( \delta \)-mollification (weighted average) of the functions with the high frequency components suitably filtered out and leaving the low frequency components essentially unmodified.
Note that from (7) and (2)
\begin{equation}
\hat{\rho}(w) = \frac{1}{2\pi} e^{-\frac{1}{4} w^2 \delta^2}
\end{equation}
and
\begin{equation}
\hat{J}\hat{f}(w) = \hat{\rho}(w) \hat{f}(w).
\end{equation}

Mollifying (1), we have the following associated problem: For some \( \delta > 0 \), find \( J_\delta U_m(t) \) and \( J_\delta q_m(t) \) given that the mollified temperature \( J_\delta u(x, t) \equiv v(x, t) \) satisfies
\begin{equation}
\begin{aligned}
&\frac{\partial}{\partial x} v(x, t) = -\frac{1}{2} \frac{\partial}{\partial t} v(x, t), \quad x > 0, \ t \geq 0, \\
v(x_1, t) = J_\delta f_m(t), \quad \text{data, } x_1 > 0, \ t > 0, \\
v(0, t) = J_\delta U_m(t), \quad \text{unknown, } t \geq 0, \\
-\frac{\partial}{\partial x} v(0, t) = J_\delta q_m(t), \quad \text{unknown, } t \geq 0.
\end{aligned}
\end{equation}
Here the unknown functions \( U_m \) and \( q_m \) are associated with the noisy data function \( f_m \).

For the mollified problem (10) the next property holds.

**Theorem 1.** Problem (10) is formally stable with respect to perturbations in the data.

**Proof.** We only show the estimate for the boundary heat flux function. A similar estimate is also valid for the temperature boundary function.

From (6), (8) and (9) and the definition of mollification, in the frequency space we have
\begin{equation}
\hat{J}\delta q(w) - \hat{J}\delta q_m(w) = \frac{1}{2\pi} e^{(-\frac{1}{4} w^2 \delta^2)} \sqrt{1 \over w} e^{\sqrt{w} x_1} (\hat{f}(w) - \hat{f}_m(w)).
\end{equation}

Thus,
\begin{equation}
|\hat{J}\delta q(w) - \hat{J}\delta q_m(w)| \leq \frac{1}{2\pi} e^{(-\frac{1}{4} w^2 \delta^2)} \sqrt{1 \over 2} e^{\sqrt{w} x_1} |\hat{f}(w) - \hat{f}_m(w)|
\end{equation}
and
\begin{equation}
|\hat{J}\delta q(w) - \hat{J}\delta q_m(w)| \leq \frac{1}{2\pi} e^{(-\frac{1}{4} w^2 \delta^2 + |w| x_1)} |\hat{f}(w) - \hat{f}_m(w)| \\
\leq \frac{1}{2\pi} e^{(2 x_1^2 \delta^2 - 2)} |\hat{f}(w) - \hat{f}_m(w)|,
\end{equation}
which implies
\begin{equation}
\|\hat{J}\delta q - \hat{J}\delta q_m\| \leq \frac{1}{2\pi} \exp(2 x_1^2 \delta^2 - 2) \|\hat{f} - \hat{f}_m\|.
\end{equation}

By Parseval’s identity (3),
\begin{equation}
\|J\delta q - J\delta q_m\| \leq \frac{1}{2\pi} \exp(2 x_1^2 \delta^2 - 2) \|f - f_m\|.
\end{equation}

The last inequality shows that the mollified FIHCP is a formally stable problem with respect to perturbations in the data for fixed \( \delta > 0 \).

Moreover, assuming a data error bound of the form
\begin{equation}
\|f - f_m\| \leq \varepsilon,
\end{equation}
for a fixed \( \delta > 0 \), \( \|J\delta q - J\delta q_m\| \to 0 \) as \( \varepsilon \to 0 \).
3. Numerical scheme

3.1. Numerical fractional derivative

The evaluation of the Riemann–Liouville fractional derivative

\[ (D^{1/2}g)(t) = \frac{1}{\Gamma(1/2)} \frac{d}{dt} \int_0^t g(s)(t-s)^{-1/2}ds, \quad 0 \leq t \leq T, \]

can be reduced to the treatment of Caputo’s fractional derivative under mild smoothing conditions on the function \( g \). After integrating by parts,

\[ (D^{1/2}g)(t) = \frac{1}{\Gamma(1/2)} \left( \int_0^t g'(s)(t-s)^{-1/2}ds + g(0)t^{-1/2} \right), \quad 0 \leq t \leq T. \]

If the mollified data function satisfies the error bound \( \| J_\delta g - J_\delta g_m \| \leq \varepsilon \), the mollified quadrature formula introduced in \cite{7}, Theorem 2.1, Part 2, allows for the computation of the quantity \( D^{1/2}t(J_\delta g_m) \) such that

\[ \| D^{1/2}t(J_\delta g_m) - D^{1/2}t(J_g) \|_\infty \leq C \left( \frac{\varepsilon}{\delta} + k \right). \]  

(11)

when the functions are restricted to the grid points of a uniform partition, of diameter \( k \), of the interval \([0, T]\).

3.2. Space marching algorithm

We propose a simple marching method, starting at \( x = \bar{x} > 0 \). From (1) the one-step explicit backward space marching scheme is given by

\[ \text{new}(u) = u - h \frac{\partial}{\partial x} u = u + h \frac{\partial^{1/2}}{\partial t^{1/2}} u \]

and it requires the evaluation of a half-fractional time derivative at each step. Similarly, the smooth exact mollified function \( v \) can be determined with the local truncation error evaluated at some intermediate point. That is,

\[ \text{new}(v) = v + h \frac{\partial^{1/2}}{\partial t^{1/2}} v + O(h^2). \]  

(12)

To describe the numerical algorithm we need to specify some grid parameters. Let \( N_x \) and \( N_t \) be positive integers, \( h = \bar{x}/N_x, k = T/N_t, x_i = ih, i = 0, 1, \ldots, N_x, t_n = nk, n = 0, 1, \ldots, N_t \), and introduce the discrete functions

\[ R^n_i : \text{the discrete approximation to } v(ih, nk), \]

\[ W^n_i : \text{the discrete approximation to } \frac{\partial^{1/2}}{\partial t^{1/2}} v(ih, nk). \]

The space marching algorithm, with \( D^{1/2}_t \) indicating the discrete approximation to the half-fractional time derivative in (11), is defined as follows:

1. Select \( \delta_{N_x} \).
2. Perform mollification of \( f_m \) and set
   \[ R^n_{N_x} = J_{\delta_{N_x}} f_m(nk). \]
3. Perform mollified fractional differentiation in time of \( J_{\delta_{N_x}} f_m(nk) \) and set
   \[ W^n_{N_x} = D^{1/2}_t (J_{\delta_{N_x}} f_m(nk)). \]
4. Initialize \( i = N_x \). Do while \( i \geq 1 \), set
   \[ R^n_{i-1} = R^n_i + h W^n_i. \]
(a) Select $\delta_{i-1}$.
(b) Perform mollified fractional differentiation in time of $R^n_{i-1}$, set
\[ W^n_{i-1} = D_t^{1/2}(J_{\delta_{i-1}}R^n_{i-1}) . \]
(c) Set $i = i - 1$.

Remark 1. The discrete approximation for $q_n(t)$ is given by $W^n_0$.

Remark 2. For further details regarding the numerical implementation of marching mollification techniques, including automatic selection of the radii of mollification and other practical issues, see [9].

3.3. Error estimates

Denoting the error between the calculated mollified discrete function $R^n_i$ and the restriction to the grid of the mollified exact function $v(ih, nk)$ by $\Delta R^n_i = v(ih, nk) - R^n_i$, from (12) and (11) we get
\[ \Delta R^n_{N_x-1} = \Delta R^n_{N_x} + hD_t^{1/2}(\Delta R^n_{N_x}) + O(h^2) \]
\[ = \Delta R^n_{N_x} + hC\left[\frac{\Delta R^n_i}{\delta} + k\right] + O(h^2), \]
where $C$ represents a generic constant.

Hence,
\[ |\Delta R^n_{N_x-1}| \leq \left(1 + \frac{Ch}{\delta}\right)|\Delta R^n_{N_x}| + O(hk + h^2) \]
and iterating $N_x - 1$ times,
\[ |\Delta R^n_0| \leq \left(1 + \frac{Ch}{\delta}\right)^{N_x}|\Delta R^n_{N_x}| + \left[1 + \left(1 + \frac{Ch}{\delta}\right) + \cdots + \left(1 + \frac{Ch}{\delta}\right)^{N_x-1}\right]O(hk + h^2), \]
\[ \leq \left(1 + \frac{Ch}{\delta}\right)^{N_x}O(hk + h^2), \]
\[ \leq e^{C\frac{Nh}{\delta}}|\Delta R^n_{N_x}| + C\delta(e^{C\frac{Nh}{\delta}} - 1)O(k + h) \]
with $h$ small enough to ensure $Ch/\delta < 1$.

Consequently,
\[ |\Delta R^n_0| \leq e^{C\frac{Nh}{\delta}}|\Delta R^n_{N_x}| + C(\delta)O(k + h) \]
and defining $|\Delta R_i| = \max_{0 \leq n \leq N_t} |\Delta R^n_i|$, $i = 0, 1, \ldots, N_x$, we have
\[ |\Delta R_0| \leq e^{C\frac{Nh}{\delta}}|\Delta R_{N_x}| + C(\delta)O(k + h). \]

Note that $|\Delta R_{N_x}| \leq \varepsilon$. Thus, for fixed $\delta$, as $\varepsilon$, $h$, and $k$ tend to 0 then so does $|\Delta R_0|$. Therefore the numerical marching scheme is formally convergent.

4. Numerical example

For linear heat diffusion, analytical solutions for the temperature distribution $u(x, t)$, $x > 0$, $t > 0$ in a semi-infinite solid with zero initial temperature and $u(0, t) = U(t)$ at the surface, are obtained using the integral equation
\[ u(x, t) = \left(U \ast \frac{\partial}{\partial t}K\right)(x, t) = \int_0^t U(s)\frac{\partial}{\partial t}K(x, t - s)\, ds \]
where the kernel function

$$K(x, t) = \text{erfc} \left( \frac{x}{2\sqrt{t}} \right)$$  (13)

is the temperature distribution corresponding to a unit step boundary temperature, $U(t) = 1, t > 0$. It is seen from (13) that in this case the interior heat flux is given by

$$-\frac{\partial}{\partial x} K(x, t) = \frac{e^{-x^2/4t}}{\sqrt{\pi}\sqrt{t}}$$

and the surface heat flux by

$$-\frac{\partial}{\partial x} K(0, t) = \frac{1}{\sqrt{\pi}\sqrt{t}}.$$

As an interesting and challenging test for the numerical method we proposed to approximately identify the surface heat flux function $q(t)$ and the surface temperature function $U(t)$, which is 1 between 0.2 and 0.6 and zero otherwise, from noisy measurements at the interior location $x = x_1 = 0.5$.

Mathematically, the FIHCP, with $T = 1$, is described as

$$\frac{\partial}{\partial x} u(x, t) = -\frac{\partial^{1/2}}{\partial t^{1/2}} u(x, t), \quad x > 0, t \geq 0,$$

$$u(0.5, t) = f_m(t), \quad \text{data, } 0 \leq t \leq 1,$$

$$u(0, t) = U_m(t), \quad \text{unknown, } 0 \leq t \leq 1,$$

$$-\frac{\partial}{\partial x} u(0, t) = q_m(t), \quad \text{unknown, } 0 \leq t \leq 1,$$

where the exact interior data temperature is given by

$$f(t) = \text{erfc} \left( \frac{0.5}{2\sqrt{t} - 0.2} \right) - \text{erfc} \left( \frac{0.5}{2\sqrt{t} - 0.6} \right).$$

The exact solutions for the FICHP, in this example, are the functions

$$u(0, t) = U(t) = \begin{cases} 1, & 0.2 < t < 0.6, \\ 0, & \text{otherwise,} \end{cases}$$

and

$$-\frac{\partial}{\partial x} K(0, t) = q(t) = \frac{1}{\sqrt{\pi}} \left( \frac{1}{\sqrt{t} - 0.2} - \frac{1}{\sqrt{t} - 0.6} \right).$$

The noisy discrete data function is generated by adding random errors to the exact data function, at every grid point, i.e.,

$$f_m(nk) = f(nk) + \epsilon_n, \quad |\epsilon_n| \leq \epsilon, \ n = 0, 1, \ldots, N_t,$$

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

The relative weighted $l^2$ errors for the recovered boundary temperatures are calculated as

$$\left[ \frac{1}{(N_t+1)} \sum_{n=0}^{N_t} |R^n_0 - u(0, nk)|^2 \right]^{1/2}$$

$$\left[ \frac{1}{(N_t+1)} \sum_{n=0}^{N_t} |u(0, nk)|^2 \right]^{1/2}$$

and their averages after 10 trials are reported in Table 1 as a function of $\epsilon$ and as a function of $N_t$ in Table 2. Both these results and those shown in Figs. 1 through 4 emphasize the stability and consistency of the marching scheme.
Fig. 1. Noisy and computed data temperatures at $x = 0.5$.

Fig. 2. Exact and computed temperatures and heat fluxes at $x = 0.5$.

Table 1
Reconstructed temperature errors

<table>
<thead>
<tr>
<th>$\epsilon$</th>
<th>Rel. $L^2$ errors for $u(0, t)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.01</td>
<td>0.11520</td>
</tr>
<tr>
<td>0.05</td>
<td>0.13734</td>
</tr>
<tr>
<td>0.10</td>
<td>0.19704</td>
</tr>
</tbody>
</table>

For Table 1 and Figs. 1–4, $N_x = 100$ and $N_t = 128$. In Table 2 and Figs. 1–4, $\epsilon = 0.05$ (about 8% level of noise in the experimental data). Note that the pictures include different scales and the computed solution is always indicated with a dashed line.
Table 2
Reconstructed temperature errors

<table>
<thead>
<tr>
<th>$N_t$</th>
<th>Rel. $l^2$ errors for $u(0,t)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>064</td>
<td>0.14119</td>
</tr>
<tr>
<td>128</td>
<td>0.13734</td>
</tr>
<tr>
<td>256</td>
<td>0.11809</td>
</tr>
</tbody>
</table>

Fig. 3. Exact and computed temperatures and heat fluxes at $x = 0.3$.

Fig. 4. Exact and computed temperatures and heat fluxes at $x = 0.0$.

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References