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Determination of order in fractional diffusion equation

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Abstract. We prove formulae of reconstructing the order of fractional derivative in time in the fractional diffusion equation by time history at one fixed spatial point. The proof is based on asymptotics of the solution as $t \to 0$ or $t \to \infty$. The order is important for evaluating the anomaly of the diffusion in heterogeneous medium, and in particular, the order determines the decay rate of solution for large t. We show numerical tests for our reconstruction formula.

Keywords. fractional diffusion equation, order of fractional derivative, inverse problem, reconstruction formula, error analysis

1. Introduction

Recently anomalous diffusion phenomena have attracted great attention, which show different aspects from the classical diffusion. For example, Adams and Gelhar [1] pointed that observation data in the saturated zone of an actual aquifer deviate from simulated results by the classical advection-diffusion equation. Some anomalous diffusion can be interpreted as slow diffusion, and is characterized by the long-tailed profile in spatial distribution of densities as the time passes. Also see Berkowitz, Cortis, Dentz and Scher [4].

For the anomalous diffusion, a microscopic model was proposed by the continuous-time random walk. That is, let $x(t)$, $t > 0$ be the probability density function of location of particle at time t, and let us assume that the mean square displacement grows as

$$\langle x^2(t)\rangle \sim t^\alpha, \tag{1.1}$$

where $\alpha > 0$ is a constant (e.g., Metzler and Klafter [14], Sokolov, Klafter and Blumen [19]). The case $\alpha = 1$ corresponds to the classical diffusion, and the transport phenomenon exhibits sub-diffusion for $\alpha < 1$, while super-diffusion for $\alpha > 1$. Thus the determination of α is needed for suitable simulation of the anomalous diffusion and there are many column experiments on reactive flow in heterogeneous media (e.g., Hatano and Hatano [9]). On the other hand, the anomalous diffusion subject to (1.1) can be described by a macroscopic model (e.g., [14, 19]) which is called a fractional diffusion equation. Here we consider a simplified form:

$$\partial_t^\alpha u(x,t) = \Delta u(x,t), \quad x \in \Omega, \tag{1.2}$$

where $\Omega \subset \mathbb{R}^d$, and we set

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

where $\Gamma(1-\alpha)$ is the gamma function. Then $u(x,t)$ describes the probability of finding a particle at location x and time t.

First we discuss the asymptotic behavior of $u(x,t)$ to clarify the slow diffusion by comparing with other model equations. First we consider

$$\partial_t^\alpha u = \Delta u, \quad x \in \mathbb{R}^d,\ t > 0. \tag{1.3}$$

Henceforth by $p(x,y,t)$ we denote the fundamental solution to the corresponding equation, and for two functions f and g in y, we understand by $f \sim g$ that there exists a constant $C > 0$ such that $C^{-1}f(y) \le g(x) \le Cf(y)$ for all y under consideration. Moreover let C, C_k denote positive constants. Then for example by (3.7) in Eidelman and Kocubei [7], we have

$$p(x,y,t) = \pi^{-\frac{d}{2}}|x-y|^{-d}H_{12}^{20}\left[\frac{|x-y|^2}{4t^\alpha}\ \begin{array}{|l} (1,\alpha) \\ \left(\frac{d}{2},1\right),\quad (1,1)\end{array}\right]$$
$$\sim C_0|x-y|^{-\frac{d(1-\alpha)}{2-\alpha}}t^{\frac{-\alpha d}{2(2-\alpha)}}\exp\left(-C_1\left(\frac{|x-y|^{\frac{2}{\alpha}}}{t}\right)^{\frac{1}{\frac{2}{\alpha}-1}}\right),$$
$$\text{as } \frac{|x-y|^2}{t^\alpha} \to \infty. \tag{1.4}$$

Here H is the H-function (see Kilbas, Srivastava and Trujillo [11], Podlubny [15]).

Next we will consider the classical diffusion equation, that is, $\alpha = 1$:

$$\partial_t u(x,t) = \Delta u(x,t), \quad x \in \mathbb{R}^d,\ t > 0.$$

Then

$$p(x,y,t) \sim t^{-\frac{d}{2}}\exp\left(-C_2\left(\frac{|x-y|^2}{t}\right)\right) \tag{1.5}$$

(see e.g., Davies [6]). Finally as diffusion process on a fractal, we discuss $\partial_t - \Delta$ on the Sierpinski gasket E. We know

$$p(x,y,t) \sim t^{-\frac{d_s}{2}} \exp\left(-C_3\left(\frac{|x-y|^{d_w}}{t}\right)^{\frac{1}{d_w-1}}\right),$$
$$x, y \in E,\ 0 < t < 1 \quad (1.6)$$

(e.g., Barlow and Perkins [3]). Here

$$d_s = \frac{2\log 3}{\log 5}: \quad \text{the spectral dimension}$$
$$d_w = \frac{\log 5}{\log 2} > 2: \quad \text{the walk dimension.}$$

Also we refer to Kigami [10] and Kumagai [12].

If $0 < \alpha < 1$, then the aymptotic behavior (1.4) essentially differs from (1.5) and (1.6) because of the factor $|x-y|^{-\frac{d(1-\alpha)}{2-\alpha}}$. This factor means that some singularity at x remains for positive time $t > 0$ of the fundamental solution which has singularity at x at time $t = 0$. This means that particles cannot diffuse rapidly, which can explain as a character of the slow diffusion. On the other hand, the asymptotic formulae (1.5) and (1.6) mean that for classical diffusion equation and the diffusion process on Sierpinski gasket, no singulariy at x appear for positive t by immediate diffusion.

Thus $\alpha \in (0,1)$ is an important index characterizing the slow diffusion. In this paper, we discuss determination of α, and establish formulae of determining $0 < \alpha < 1$ by observation data $u(x_0,t)$, $t > 0$ with fixed $x_0 \in \Omega$. Our formulae may give easy way for determining α, e.g., by experiments in the flow cells or columns. This paper is composed of five sections. In Section 2 we show main results and Section 3 is devoted to the proof. In Section 4 we discuss an error analysis of the formula at $t \to 0$ for noisy data and in Section 5, we make numerical testing.

2. Main result

Consider

$$\partial_t^\alpha u(x,t) = (Lu)(x,t)$$
$$\equiv \sum_{i,j=1}^d \frac{\partial}{\partial x_i}\left(a_{ij}(x)\frac{\partial u}{\partial x_j}\right) + c(x)u(x,t),$$
$$x \in \Omega,\ 0 < t < T, \qquad (2.1)$$
$$\partial_L u(x,t) + \sigma(x)u(x,t) = 0, \qquad x \in \partial\Omega,\ 0 < t < T,$$

and

$$u(x,0) = a(x), \qquad x \in \Omega.$$

Here $\Omega \subset \mathbb{R}^d$ is a bounded domain with smooth boundary $\partial\Omega$, $\nu(x) = (\nu_1(x), \ldots, \nu_d(x))$ denotes the unit outward normal vector to $\partial\Omega$ at x and a_{ij}, c are sufficiently smooth. Moreover $a_{ij} = a_{ji}$, $1 \le i,j \le d$ are of $C^1(\overline{\Omega})$, $c \in C(\overline{\Omega})$, $c(x) \le 0$ for $x \in \Omega$, $\sigma \in C^\infty(\partial\Omega)$, ≥ 0, $\not\equiv 0$ on $\partial\Omega$, there exists a constant $\nu > 0$ such that

$$\sum_{i,j=1}^d a_{ij}(x)\xi_i\xi_j \ge \nu \sum_{j=1}^d \xi_j^2, \qquad x \in \Omega,\ \xi_1, \ldots, \xi_d \in \mathbb{R},$$

and we set

$$\partial_L v(x) = \sum_{i,j=1}^d a_{ij}(x)\frac{\partial v}{\partial x_j}(x)\nu_i(x), \quad x \in \partial\Omega.$$

Inverse Problem. Let $x_0 \in \Omega$ be fixed. Determine $\alpha \in (0,1)$ from observation data

$$u(x_0,t) \qquad \text{for small } t \text{ or large } t.$$

Theorem 1. (i) *We assume that*

$$a \in C_0^\infty(\Omega), \quad La(x_0) \ne 0.$$

Then

$$\alpha = \lim_{t\to 0} \frac{t\frac{\partial u}{\partial t}(x_0,t)}{u(x_0,t) - a(x_0)}. \qquad (2.2)$$

(ii) *We assume that*

$$a \in C_0^\infty(\Omega), \quad a \ge 0 \text{ or } \le 0,\ \not\equiv 0 \text{ on } \overline{\Omega}.$$

Then

$$\alpha = -\lim_{t\to\infty} \frac{t\frac{\partial u}{\partial t}(x_0,t)}{u(x_0,t)}. \qquad (2.3)$$

Remark 1. (i) gives an identification formula for the order α by data near $t = 0$, while (ii) is for data for large $t > 0$. The condition $a \in C_0^\infty(\Omega)$ means that $a = 0$ near the boundary $\partial\Omega$ and a is infinitely many times differentiable in Ω. For example we can take a very smooth bell-shaped function as $a(x)$.

As is seen from the proof in section 3, we see the following: for any fixed small $\delta > 0$, there exists a constant $C_0 > 0$ depending on a_{ij}, c, a, Ω, σ, such that

$$\left|\left(-\frac{T\frac{\partial u}{\partial t}(x_0,T)}{u(x_0,T)}\right) - \alpha\right| \le \frac{C_0}{T^\alpha}$$

for any $\alpha \in [0, 1-\delta]$. This is useful for estimating errors when we approximate α by setting $t = T$:

$$-\frac{T\frac{\partial u}{\partial t}(x_0,T)}{u(x_0,T)}.$$

3. Proof of Theorem 1

Let $L^2(\Omega)$, $H^\ell(\Omega)$, $\ell \in \mathbb{N}$, denote usual Lebesgue space and Sobolev space and let us set

$$(a,b) = \int_\Omega a(x)b(x)\,dx, \quad \|a\| = (a,a)^{\frac{1}{2}}.$$

Let $\{\varphi_n\}_{n\in\mathbb{N}}$ be the set of all the eigenfunctions of L with the boundary condition $\partial_L u + \sigma u = 0$; that is, $L\varphi_n = -\lambda_n\varphi_n$, $\varphi_n \ne 0$, and $\partial_L\varphi_n(x) + \sigma(x)\varphi_n(x) = 0$ for $x \in \partial\Omega$. Here and henceforth we number the eigenvalues with multiplicities as

$$\lambda_1 \le \lambda_2 \le \cdots,$$

and we choose φ_n such that $(\varphi_n, \varphi_n) = 1$ and $(\varphi_n, \varphi_m) = 0$ if $n \neq m$. Then we can prove

$$\lambda_n > 0, \qquad n \in \mathbb{N}.$$

In fact, $\lambda_n \geq 0$ can be first proved as follows. Let $Lu = -\lambda_n u$, $\partial_L u + \sigma u = 0$ and $u \not\equiv 0$. Then, multiplying $Lu = \lambda_n u$ by u and integrating by parts, and using the boundary condition, $\sigma \geq 0$ and $c \leq 0$, we obtain

$$\begin{aligned}
&-\lambda_n \|u\|^2 \\
&= \int_\Omega \left(\sum_{i,j=1}^d \frac{\partial}{\partial x_i}\left(a_{ij}\frac{\partial u}{\partial x_j}\right) + cu \right) u\,dx \\
&= \int_\Omega \left(-\sum_{i,j=1}^d a_{ij}\frac{\partial u}{\partial x_i}\frac{\partial u}{\partial x_j} + cu^2 \right) dx + \int_{\partial\Omega} (\partial_L u) u\,dS \\
&= \int_\Omega \left(-\sum_{i,j=1}^d a_{ij}\frac{\partial u}{\partial x_i}\frac{\partial u}{\partial x_j} + cu^2 \right) dx - \int_{\partial\Omega} \sigma u^2\,dS \\
&\leq 0.
\end{aligned}$$

Therefore by $u \not\equiv 0$, we see that $\lambda_n \geq 0$. Moreover let $Lu_0 = 0$ in Ω and $\partial_L u_0 + \sigma u_0 = 0$ on $\partial\Omega$. Then by the above equalities, we have

$$\int_\Omega \left(-\sum_{i,j=1}^d a_{ij}\frac{\partial u_0}{\partial x_i}\frac{\partial u_0}{\partial x_j} + cu_0^2 \right) dx - \int_{\partial\Omega} \sigma u_0^2\,dS = 0,$$

which implies $\nabla u_0 = 0$ in Ω. Hence u_0 is a constant function, and $\int_{\partial\Omega} \sigma u_0^2\,dS = 0$. Since $\sigma \not\equiv 0$ on $\partial\Omega$, we see that $u_0 = 0$. This means that 0 can not be an eigenvalue. Thus we have proved that $\lambda_n > 0$, $n \in \mathbb{N}$.

By $a \in C_0^\infty(\Omega)$, we can see the following: For any $\ell \in \mathbb{N}$, there exists a constant $C(\ell) > 0$ such that

$$|(a, \varphi_n)| \leq \frac{C(\ell)}{|\lambda_n|^\ell}, \qquad n \in \mathbb{N} \tag{3.1}$$

and

$$\begin{aligned}
\sum_{n=1}^\infty -\lambda_n (a, \varphi_n)\varphi_n(x_0) &= La(x_0), \\
\sum_{n=1}^\infty (a, \varphi_n)\varphi_n(x_0) &= a(x_0).
\end{aligned} \tag{3.2}$$

Moreover $L\varphi_n = -\lambda_n\varphi_n$ in Ω implies $\|L^m\varphi_n\| = |\lambda_n|^m$, $m \in \mathbb{N}$. By the regularity of elliptic equation (e.g., Gilbarg and Trudinger [8]), we see that there exists a constant $C_1 > 0$ such that $\|\varphi_n\|_{H^{2m}(\Omega)} \leq C_1(\|L^m\varphi_n\| + \|\varphi_n\|)$. Here $\|\varphi_n\|_{H^{2m}(\Omega)}$ is the norm in $H^{2m}(\Omega)$ (e.g., Adams [2]). By the Sobolev embedding theorem (e.g., [2]), if $m > \frac{d}{4}$, then there exists a constant $C_2 = C_2(m) > 0$ such that

$$\max_{x \in \overline{\Omega}} |\varphi_n(x)| \leq C_2 \|\varphi_n\|_{H^{2m}(\Omega)} \leq C_1 C_2 (|\lambda_n|^m + 1), \quad n \in \mathbb{N}.$$

Hence there exist constants $\kappa > 0$ and $C_3 > 0$ such that

$$|\varphi_n(x_0)| \leq C_3 |\lambda_n|^\kappa, \quad n \in \mathbb{N}. \tag{3.3}$$

Moreover

$$|\lambda_n| \leq C_4 n^{\frac{2}{d}} \tag{3.4}$$

(e.g., Courant and Hilbert [5]). Therefore, by (3.1)–(3.3), similarly to Sakamoto and Yamamoto [18], by the Fourier method, we can prove

$$u(x_0, t) = \sum_{n=1}^\infty (a, \varphi_n)\varphi_n(x_0) E_{\alpha,1}(-\lambda_n t^\alpha), \ 0 < t < T, \tag{3.5}$$

where the series is convergent in $C[0, T]$. Here the Mittag-Leffler function is defined as follows:

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

(e.g., Podlubny [15]). Therefore

$$\begin{aligned}
\frac{\partial u}{\partial t}(x_0, t) &= \sum_{n=1}^\infty (a, \varphi_n)\varphi_n(x_0) \frac{d}{dt} E_{\alpha,1}(-\lambda_n t^\alpha) \\
&= \sum_{n=1}^\infty -\lambda_n (a, \varphi_n)\varphi_n(x_0) t^{\alpha-1} E_{\alpha,\alpha}(-\lambda_n t^\alpha), \\
&\qquad 0 < t < T
\end{aligned} \tag{3.6}$$

(e.g., formula (1.83) on p. 22 in [15]). On the other hand,

$$\begin{aligned}
E_{\alpha,\alpha}(-\lambda_n t^\alpha) &= \sum_{k=0}^\infty \frac{(-\lambda_n t^\alpha)^k}{\Gamma((k+1)\alpha)} \\
&= \frac{1}{\Gamma(\alpha)} + t^\alpha \left(\frac{E_{\alpha,\alpha}(-\lambda_n t^\alpha) - \Gamma(\alpha)^{-1}}{t^\alpha} \right) \\
&\equiv \frac{1}{\Gamma(\alpha)} + t^\alpha r_n(t),
\end{aligned}$$

where $r_n(t)$ is continuous at $t = 0$ and $\lim_{t\to 0} r_n(t)$ exists. Hence

$$\begin{aligned}
\frac{\partial u}{\partial t}(x_0, t) &= \left(\sum_{n=1}^\infty -\lambda_n (a, \varphi_n)\varphi_n(x_0) \right) \frac{t^{\alpha-1}}{\Gamma(\alpha)} \\
&\quad + \left(\sum_{n=1}^\infty -\lambda_n (a, \varphi_n)\varphi_n(x_0) r_n(t) \right) t^{2\alpha-1},
\end{aligned}$$

and

$$\begin{aligned}
&\lim_{t\to 0} t^{1-\alpha} \frac{\partial u}{\partial t}(x_0, t) \\
&\quad = \frac{1}{\Gamma(\alpha)} \left(\sum_{n=1}^\infty -\lambda_n (a, \varphi_n)\varphi_n(x_0) \right) \\
&\qquad + \lim_{t\to 0} t^\alpha \left(\sum_{n=1}^\infty -\lambda_n (a, \varphi_n)\varphi_n(x_0) r_n(t) \right).
\end{aligned} \tag{3.7}$$

By [15] (formula (1.148) on p. 35), we have

$$\begin{aligned}
|r_n(t)| &= \left| \sum_{k=1}^\infty \frac{(-\lambda_n)^k t^{\alpha(k-1)}}{\Gamma((k+1)\alpha)} \right| = |\lambda_n| \left| \sum_{k=0}^\infty \frac{(-\lambda_n t^\alpha)^k}{\Gamma(k\alpha + 2\alpha)} \right| \\
&= |\lambda_n| |E_{\alpha,2\alpha}(-\lambda_n t^\alpha)| \leq |\lambda_n|, \qquad t \geq 0,\ n \in \mathbb{N}.
\end{aligned}$$

Hence, by (3.1) and (3.3),

$$\left|\sum_{n=1}^{\infty} -\lambda_n (a,\varphi_n)\varphi_n(x_0) r_n(t)\right| \le \sum_{n=1}^{\infty} |\lambda_n|^2 |(a,\varphi_n)\varphi_n(x_0)| \le \sum_{n=1}^{\infty} |\lambda_n|^2 \frac{C(\ell)}{|\lambda_n|^\ell} C_3 |\lambda_n|^\kappa.$$

By (3.4), we take sufficiently large $\ell \in \mathbb{N}$ to have

$$\max_{0\le t\le T}\left|\sum_{n=1}^{\infty} -\lambda_n (a,\varphi_n)\varphi_n(x_0) r_n(t)\right| < \infty. \tag{3.8}$$

Hence, by using (3.2), equation (3.7) yields

$$\lim_{t\to 0} t^{1-\alpha}\frac{\partial u}{\partial t}(x_0,t) = \frac{La(x_0)}{\Gamma(\alpha)}. \tag{3.9}$$

On the other hand, we have

$$\begin{aligned} E_{\alpha,1}(-\lambda_n t^\alpha) &= 1 - \frac{\lambda_n t^\alpha}{\Gamma(\alpha+1)} + t^{2\alpha}\sum_{k=2}^{\infty}\frac{(-\lambda_n)^k t^{\alpha(k-2)}}{\Gamma(\alpha k+1)} \\ &= 1 - \frac{\lambda_n t^\alpha}{\Gamma(\alpha+1)} + t^{2\alpha}\lambda_n^2 E_{\alpha,2\alpha+1}(-\lambda_n t^\alpha). \end{aligned}$$

Therefore, using (3.2), we have

$$\begin{aligned} u(x_0,t) &= \sum_{n=1}^{\infty}(a,\varphi_n)\varphi_n(x_0) + \sum_{n=1}^{\infty}\frac{-\lambda_n(a,\varphi_n)\varphi_n(x_0)}{\Gamma(\alpha+1)} t^\alpha \\ &\quad + t^{2\alpha}\sum_{n=1}^{\infty}\lambda_n^2 E_{\alpha,2\alpha+1}(-\lambda_n t^\alpha)(a,\varphi_n)\varphi_n(x_0) \\ &= a(x_0) + \frac{La(x_0)}{\Gamma(\alpha+1)} t^\alpha + t^{2\alpha}\widetilde{r}(t). \end{aligned}$$

Here by (3.1), we see that $\sup_{0\le t\le T}|\widetilde{r}(t)| < \infty$. Consequently

$$\lim_{t\to 0} t^{-\alpha}(u(x_0,t) - a(x_0)) = \frac{La(x_0)}{\Gamma(\alpha+1)}. \tag{3.10}$$

In terms of (3.9) and (3.10), using $La(x_0) \ne 0$ and $\Gamma(\alpha+1) = \alpha\Gamma(\alpha)$, we have

$$\lim_{t\to 0}\frac{t\frac{\partial u}{\partial t}(x_0,t)}{u(x_0,t)-a(x_0)} = \frac{\lim_{t\to 0} t^{1-\alpha}\frac{\partial u}{\partial t}(x_0,t)}{\lim_{t\to 0} t^{-\alpha}(u(x_0,t)-a(x_0))} = \frac{\frac{La(x_0)}{\Gamma(\alpha)}}{\frac{La(x_0)}{\Gamma(\alpha+1)}} = \alpha.$$

Thus we can complete the proof of (i).

Next we will prove (ii). In (3.5) and (3.6), we apply the asymptotic behavior of the Mittag-Leffler function at ∞ (e.g., Theorem 1.4 (pp. 33–34) in [15]):

$$E_{\alpha,1}(-\eta) = \frac{\eta^{-1}}{\Gamma(1-\alpha)} + O\left(\frac{1}{\eta^2}\right)$$

and

$$E_{\alpha,\alpha}(-\eta) = -\frac{\eta^{-2}}{\Gamma(-\alpha)} + O\left(\frac{1}{\eta^3}\right)$$

as $\eta \to \infty$, $\eta > 0$. Therefore

$$u(x_0,t) = \sum_{n=1}^{\infty}(a,\varphi_n)\varphi_n(x_0)\frac{1}{\Gamma(1-\alpha)\lambda_n t^\alpha} + O\left(\frac{1}{t^{2\alpha}}\right)\sum_{n=1}^{\infty}(a,\varphi_n)\varphi_n(x_0)\frac{1}{\lambda_n^2}$$

and

$$\frac{\partial u}{\partial t}(x_0,t) = \sum_{n=1}^{\infty}(a,\varphi_n)\varphi_n(x_0)\frac{1}{\Gamma(-\alpha)\lambda_n t^{\alpha+1}} + O\left(\frac{1}{t^{2\alpha+1}}\right)\sum_{n=1}^{\infty}(a,\varphi_n)\varphi_n(x_0)\frac{1}{\lambda_n^2}.$$

Since $L\varphi_n = -\lambda_n\varphi_n$ in Ω, noting that $\lambda_n > 0$, we see that

$$\sum_{n=1}^{\infty}\frac{(a,\varphi_n)\varphi_n(x_0)}{\lambda_n} = -(L^{-1}a)(x_0),$$
$$\sum_{n=1}^{\infty}\frac{(a,\varphi_n)\varphi_n(x_0)}{\lambda_n^2} = (L^{-2}a)(x_0),$$

we obtain

$$u(x_0,t) = \frac{-(L^{-1}a)(x_0)}{\Gamma(1-\alpha)t^\alpha} + O\left(\frac{1}{t^{2\alpha}}\right)(L^{-2}a)(x_0)$$

and

$$\frac{\partial u}{\partial t}(x_0,t) = \frac{-(L^{-1}a)(x_0)}{\Gamma(-\alpha)t^{\alpha+1}} + O\left(\frac{1}{t^{2\alpha+1}}\right)(L^{-2}a)(x_0).$$

Here we can prove

$$(L^{-1}a)(x_0) \ne 0.$$

In fact, we set $b(x) = L^{-1}a(x)$, $x \in \Omega$. Then $Lb(x) = a(x)$, $x \in \Omega$. Without loss of generality, we may assume that $a \ge 0$ on $\overline{\Omega}$. Then $Lb(x) \ge 0$ in Ω. By the strong maximum principle (e.g., Theorem 4.10 (p. 109) in Renardy and Rogers [17]), in view of $c \le 0$ on $\overline{\Omega}$, we see that $\max_{x\in\overline{\Omega}} b(x) < 0$, which means $L^{-1}a(x_0) \ne 0$.

Therefore

$$\frac{t\frac{\partial u}{\partial t}(x_0,t)}{u(x_0,t)} = \frac{\frac{-(L^{-1}a)(x_0)}{\Gamma(-\alpha)t^\alpha} + O\left(\frac{1}{t^{2\alpha}}\right)(L^{-2}a)(x_0)}{\frac{-(L^{-1}a)(x_0)}{\Gamma(1-\alpha)t^\alpha} + O\left(\frac{1}{t^{2\alpha}}\right)(L^{-2}a)(x_0)} \longrightarrow \frac{\Gamma(1-\alpha)}{\Gamma(-\alpha)}$$

as $t \to \infty$. Since $\Gamma(1-\alpha) = -\alpha\Gamma(-\alpha)$, the proof of (ii) is completed.

Remark 2. By (3.5) and (3.6), we can approximate $u(x_0,t)$ and $\frac{\partial u}{\partial t}(x_0,t)$ by the N-partial sums

$$u_N(t) = \sum_{n=1}^{N}(a,\varphi_n)\varphi_n(x_0)E_{\alpha,1}(-\lambda_n t^\alpha)$$

and

$$v_N(t) = \sum_{n=1}^{N}(a, \varphi_n)\varphi_n(x_0)\frac{d}{dt}E_{\alpha,1}(-\lambda_n t^\alpha)$$

respectively. Since $E_{\alpha,1}(-\lambda_n t^\alpha)$ is completely monotonic (e.g., Pollard [16]), we see that

$$\frac{d}{dt}E_{\alpha,1}(-\lambda_n t^\alpha) \le 0, \quad \frac{d^2}{dt^2}E_{\alpha,1}(-\lambda_n t^\alpha) \ge 0, \quad t \ge 0.$$

Therefore $u_N(t)$ and $v_N(t)$ are linear combinations of monotone decreasing functions and monotone increasing functions respectively. Thus we can assume that $\frac{tv_n(t)}{u_N(t)}$ which is a truncated formula of (2.3), does not oscillate tremendously as $t \to \infty$.

4. Error estimate with noisy data

We discuss formula (2.2) in the case where available data $d(t)$ are polluted with errors in C^1. Here we give only a sketch and in a forthcoming paper we will discuss details in the case of errors in L^2, which is more realistic. Henceforth C_k denote generic constants which are independent of t and α, δ and dependent on γ, t_0. For the formulation, we assume to be given a priori bounds $\gamma \in (0,1)$ and $\delta > 0$ such that

$$0 < \alpha < \gamma < 1 \tag{4.1}$$

and

$$\left|d'(t) - \frac{\partial u}{\partial t}(x_0,t)\right| \le C_1\delta t^{\gamma-1}, \quad 0 \le t \le t_0, \quad d(0) = a(x_0). \tag{4.2}$$

Here and henceforth we set $\eta'(t) = \frac{d\eta}{dt}(t)$ and assume that $t_0 > 0$ is small.

We note that $\delta > 0$ is a noise level and we have to consider the factor $t^{\gamma-1}$ in (4.2). Because we can prove

$$\left|\frac{\partial u}{\partial t}(x_0,t)\right| \sim t^{\alpha-1} \tag{4.3}$$

as $t \to 0$ for $a \in C_0^\infty(\Omega)$ (e.g., [18]) and so we have to take into consideation the singularity at $t = 0$ also for available data. Moreover we notice that

$$\left|\frac{\partial u}{\partial t}(x_0,t)\right| \le C_1\delta t^{\gamma-1} \le C_2\delta t^{\alpha-1}$$

by $\alpha \le \gamma$ and $0 \le t \le t_0$.

We prove an error estimate under conditons (4.1) and (4.2).

Proposition 1. *We assume*

$$a \in C_0^\infty(\Omega), \quad La(x_0) \ne 0.$$

Then

$$\limsup_{t\downarrow 0}\left|\frac{t\frac{\partial u}{\partial t}(x_0,t)}{u(x_0,t)-a(x_0)} - \frac{td'(t)}{d(t)-a(x_0)}\right| \le C_1\delta\left(\frac{1}{|La(x_0)|} + \frac{1}{|La(x_0)|(|La(x_0)| - C_1\delta)}\right).$$

Since $La(x_0) \ne 0$, we see that

$$\limsup_{t\downarrow 0}\left|\frac{t\frac{\partial u}{\partial t}(x_0,t)}{u(x_0,t)-a(x_0)} - \frac{td'(t)}{d(t)-a(x_0)}\right| = O(\delta).$$

Proof. For simplicity we set $a_0 = a(x_0)$ and $a_1 = La(x_0)$. First we prove

$$u(x_0,t) - a_0 = \frac{t^\alpha}{\Gamma(\alpha+1)}a_1 + t^{2\alpha}r(t), \quad 0 \le t \le t_0, \tag{4.4}$$

where $|r(t)| \le C_2$ for $0 \le t \le t_0$. In fact, by [18] for example, we have

$$\begin{aligned}
&u(x_0,t) - a_0 \\
&= \sum_{n=1}^\infty (a,\varphi_n)E_{\alpha,1}(-\lambda_n t^\alpha)\varphi_n(x_0) - \sum_{n=1}^\infty (a,\varphi_n)\varphi_n(x_0) \\
&= \sum_{n=1}^\infty (a,\varphi_n)(E_{\alpha,1}(-\lambda_n t^\alpha) - 1)\varphi_n(x_0) \\
&= \sum_{n=1}^\infty (a,\varphi_n)\frac{-\lambda_n t^\alpha}{\Gamma(\alpha+1)}\varphi_n(x_0) \\
&\quad + \sum_{n=1}^\infty (a,\varphi_n)\left(E_{\alpha,1}(-\lambda_n t^\alpha) - 1 + \frac{\lambda_n t^\alpha}{\Gamma(\alpha+1)}\right)\varphi_n(x_0) \\
&= \frac{t^\alpha}{\Gamma(\alpha+1)}a_1 + t^{2\alpha}\sum_{n=1}^\infty (a,\varphi_n)\lambda_n^2 E_{\alpha,2\alpha+1}(-\lambda_n t^\alpha)\varphi_n(x_0).
\end{aligned}$$

Here we used the representation of $E_{\alpha,2\alpha+1}(-\lambda_n t^\alpha)$ by the power series.

We set

$$r(t) = \sum_{n=1}^\infty (a,\varphi_n)\lambda_n^2 E_{\alpha,2\alpha+1}(-\lambda_n t^\alpha)\varphi_n(x_0).$$

By [15] we see that $|E_{\alpha,2\alpha+1}(-\lambda_n t^\alpha)| \le C_3$ for $t \ge 0$, and so

$$|r(t)| \le C_4\sum_{n=1}^\infty |(a,\varphi_n)\lambda_n^2\varphi_n(x_0)|.$$

By $a \in C_0^\infty(\Omega)$, using (3.3) and (3.4), we can prove $|r(t)| \le C_5$ for $t \ge 0$ similarly to (3.8). Thus the proof of (4.4) is completed.

Therefore we have

$$|u(x_0,t) - a_0| \ge \frac{t^\alpha}{\Gamma(\alpha+1)}(a_1 - C_5 t^\alpha), \quad 0 \le t \le t_0. \tag{4.5}$$

Moreover (4.2) yields

$$|d(t) - u(x_0,t)| \le \int_0^t C_1\delta s^{\alpha-1}\,ds \le C_6 t^\alpha\delta, \quad 0 \le t \le t_0. \tag{4.6}$$

Hence (4.5) and (4.6) imply

$$\begin{aligned}
|d(t) - a_0| &= |u(x_0,t) - a_0 + d(t) - u(x_0,t)| \\
&\ge |u(x_0,t) - a_0| - |d(t) - u(x_0,t)| \\
&\ge \frac{t^\alpha}{\Gamma(\alpha+1)}(a_1 - C_5 t^\alpha) - C_6 t^\alpha\delta \\
&\ge \frac{t^\alpha}{\Gamma(\alpha+1)}(a_1 - C_7\delta - C_7 t^\alpha). \qquad (4.7)
\end{aligned}$$

Moreover (4.2) and (4.3) yield

$$\begin{aligned}|d'(t)| &\le \left|d'(t) - \frac{\partial u}{\partial t}(x_0,t)\right| + \left|\frac{\partial u}{\partial t}(x_0,t)\right| \qquad (4.8)\\ &\le C_1\delta t^{\alpha-1} + C_2 t^{\alpha-1} \le C_8 t^{\alpha-1}, \quad 0 \le t \le t_0.\end{aligned}$$

Therefore we use (4.2), (4.5) and (4.6)–(4.8) to obtain

$$\begin{aligned}&\left|\frac{t\frac{\partial u}{\partial t}(x_0,t)}{u(x_0,t)-a(x_0)} - \frac{td'(t)}{d(t)-a(x_0)}\right|\\ &= t\frac{\left|\left(\frac{\partial u}{\partial t}(x_0,t) - d'(t)\right)(d(t)-a_0) + d'(t)(d(t)-u(x_0,t))\right|}{|(u(x_0,t)-a_0)(d(t)-a_0)|}\\ &\le t\left(\frac{\left|\frac{\partial u}{\partial t}(x_0,t)-d'(t)\right|}{|u(x_0,t)-a_0|} + \frac{|d'(t)||d(t)-u(x_0,t)|}{|(u(x_0,t)-a_0)(d(t)-a_0)|}\right)\\ &\le C_9 t\left(\frac{C_1\delta t^{\alpha-1}}{t^\alpha(a_1-C_5t^\alpha)} + \frac{C_9t^{\alpha-1}t^\alpha\delta}{t^{2\alpha}(a_1-C_5t^\alpha)(a_1-C_7\delta-C_7t^\alpha)}\right)\\ &= C_9\left(\frac{C_1\delta}{a_1-C_5t^\alpha} + \frac{C_9\delta}{(a_1-C_5t^\alpha)(a_1-C_7\delta-C_7t^\alpha)}\right).\end{aligned}$$

Thus the proof of the proposition is completed. □

5. Numerical tests

The numerical tests were performed for the following Robin-typed boundary value problem

$$\begin{cases}\dfrac{\partial^\alpha u}{\partial t^\alpha} = \dfrac{\partial^2 u}{\partial x^2}, \quad 0 < x < 10, \quad 0 < t < 2, \quad 0 < \alpha \le 1\\ u_x(0,t) = 2u(0,t), \quad u_x(10,t) = 0, \quad 0 < t < 2,\\ u(x,0) = 1, \quad 0 < x < 10.\end{cases}$$

The forward problem was solved by numerical difference method with Caputo fractional derivative of order $\alpha \in (0,1)$ and implicit scheme [13], and the numbers of the spatial grids and the temporal grids are 200 and 1000, respectively. The fractional differential order was determined by (2.2), which is a reconstruction formula by data of solution near $t = 0$ and four fractional differential orders such as $\alpha = 0.4, 0.6, 0.8, 0.9$ were tested. The results are demonstrated in Figure 1. Here for simplicity of the computations, we choose an initial value $u(x,0) = 1$, $0 < x < 10$. Although the initial value does not satisfy the conditions in the theorem, our numerical performance is quite good.

The numerical results show that the recovered value of α has the very steep deceleration at the beginning time, and then its deceleration rate is changed to very small near the expected value very quickly, therefore the fractional differential order can be easily identified from the recovery formula (2.2).

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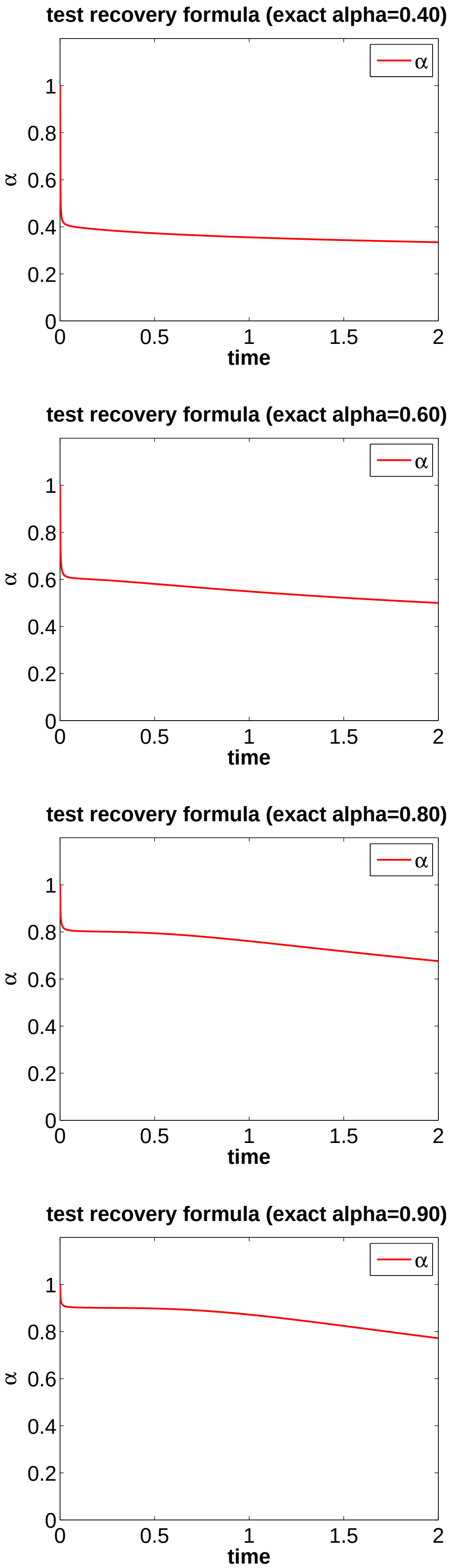

Figure 1: Recovering α from formula (2.2)

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