

INVERSE PROBLEMS FOR FRACTIONAL DIFFUSION EQUATIONS

A Dissertation

by

LIHUA ZUO

Submitted to the Office of Graduate Studies of
Texas A&M University
in partial fulfillment of the requirements for the degree of

DOCTOR OF PHILOSOPHY

Chair of Committee,	William Rundell
Committee Members,	Joe Pasciak
	Yalchin Efendiev
	Bani Mallick
Department Head,	Emil J. Straube

August 2013

Major Subject: Mathematics

Copyright 2013 Lihua Zuo

ABSTRACT

In recent decades, significant interest, based on physics and engineering applications, has developed on so-called *anomalous diffusion* processes that possess different spread functions with classical ones. The resulting differential equation whose fundamental solution matches this decay process is best modeled by an equation containing a fractional order derivative. This dissertation mainly focuses on some inverse problems for fractional diffusion equations.

After some background introductions and preliminaries in Section 1 and 2, in the third section we consider our first inverse boundary problem. This is where an unknown boundary condition is to be determined from overposed data in a time-fractional diffusion equation. Based upon the fundamental solution in free space, we derive a representation for the unknown parameters as the solution of a nonlinear Volterra integral equation of second kind with a weakly singular kernel. We are able to make physically reasonable assumptions on our constraining functions (initial and given boundary values) to be able to prove a uniqueness and reconstruction result. This is achieved by an iterative process and is an immediate result of applying a certain fixed point theorem. Numerical examples are presented to illustrate the validity and effectiveness of the proposed method.

In the fourth section a reaction-diffusion problem with an unknown nonlinear source function, which has to be determined from overposed data, is considered. A uniqueness result is proved and a numerical algorithm including convergence analysis under some physically reasonable assumptions is presented in the one-dimensional case. To show effectiveness of the proposed method, some results of numerical simulations are presented. In Section 5, we also attempted to reconstruct a nonlinear

source in a heat equation from a number of known input sources. This represents a new research even for the case of classical diffusion and would be the first step in a solution method for the fractional diffusion case. While analytic work is still in progress on this problem, Newton and Quasi-Newton method are applied to show the feasibility of numerical reconstructions.

In conclusion, the fractional diffusion equations have some different properties with the classical ones but there are some similarities between them. The classical tools like integral equations and fixed point theory still hold under slightly different assumptions. Inverse problems for fractional diffusion equations have applications in many engineering and physics areas such as material design, porous media. They are trickier than classical ones but there are also some advantages due to the mildly ill-conditioned singularity caused by the new kernel functions.

DEDICATION

To the love and support from my wife Yi Ren and my daughter Olivia.

ACKNOWLEDGEMENTS

Many thanks to my advisor, Prof. William Rundell. We first met when I was his Teaching Assistant in 2008. I was impressed by his versatile knowledge and easy-going personality. With his guidance, I have gained valuable training in doing inverse problems research. He taught me how to analyze problems and resolve difficult issues effectively and intelligently. I learned how to code and how to write a good paper. Moreover, his friendship will remain as a long-lasting memory in my mind. It is amazing to do research with such an energetic mathematician.

I was lucky to have Dr. Bangti Jin here, who is one postdoc working with Prof. Rundell. Even though we are peers (he is only two years older), his research experiences and generosity helped me a lot. Thanks to my other coauthors, Dr. Xiang Xu, Prof. Masahiro Yamamoto and Prof. Yury Luchko. They are the pioneers in my research area and they gave me much advice during our collaborations.

I express my deep gratitude to my committee members. Prof. Joe Pasciak's class on Numerical Analysis built a foundation for my computational ability. Thanks to Prof. Efendiev for introducing me to the research area of multi-scale modeling. Prof. Mallick always took time to meet with me about my research.

I am thankful to Dr. Yvette Hester, who gave me much advice on how to be a good math teacher. I thank Ms. Monique Stewart for her whole-hearted service to graduate students. Her patience in answering our trivial questions make our studies much easier. I am also thankful to the colleagues, other faculty members and staff in the Department of Mathematics of Texas A&M University. Together, they made the department a home for me for so many years. They have witnessed my growth throughout the years and will stay in my memory.

TABLE OF CONTENTS

	Page
ABSTRACT	ii
DEDICATION	iv
ACKNOWLEDGEMENTS	v
TABLE OF CONTENTS	vi
LIST OF FIGURES	ix
LIST OF TABLES	x
1. INTRODUCTION	1
1.1 Basic spaces	1
1.2 Fixed point theory	4
1.3 Volterra equation of the second kind	6
1.4 Classical diffusion equations	6
1.4.1 Derivation	7
1.4.2 Fundamental solutions	7
1.4.3 Existence and uniqueness	8
1.4.4 Regularity	9
1.4.5 Maximum principle	10
1.5 Fractional diffusion equations; preliminaries	10
1.5.1 Soil pollution	11
1.5.2 Lévy flights	11
1.5.3 Derivation of fractional diffusion equations	12
1.6 Fractional calculus	12
1.7 Mittag-Leffler function	14
1.7.1 Derivatives	15
1.7.2 Laplace transform	15
1.7.3 Asymptotic behavior	16
1.8 Wright functions	17
1.8.1 Laplace transform	18
1.8.2 Asymptotic behavior	19
2. PRELIMINARIES	20

2.1	Fractional derivatives	20
2.1.1	Riemann-Liouville derivative	20
2.1.2	Caputo derivative	21
2.1.3	Differences between two derivatives	23
2.2	New properties	24
2.2.1	Composition	24
2.2.2	Leibniz rule	24
2.3	New phenomena	25
2.3.1	Backward problem	25
2.3.2	Inverse Sturm-Liouville problem	27
2.3.3	Numerical mechanism	27
2.4	Direct solution for fractional diffusion equations	28
2.4.1	Fundamental solutions	28
2.4.2	Properties of the fundamental solution	31
2.4.3	Unique existence and regularity	36
2.4.4	Weak maximum principle	41
2.4.5	Solution for Dirichlet boundary conditions	42
2.4.6	Solution for Neumann boundary conditions	45
2.5	Numerical evaluations	47
2.5.1	Evaluation of Wright function	47
2.5.2	Finite difference scheme for fractional diffusion equations	48
2.5.3	Smoothing spline interpolation	49
3.	INVERSE BOUNDARY PROBLEMS FOR FRACTIONAL DIFFUSION EQUATIONS	51
3.1	Existence and uniqueness	55
3.2	Numerical examples	61
4.	INVERSE SOURCE PROBLEMS FOR ONE FRACTIONAL DIFFUSION EQUATION	67
4.1	Uniqueness results	68
4.2	Existence results in the one-dimensional case	73
4.3	Numerical example of reconstruction of the unknown source function	81
5.	NUMERICAL METHOD FOR RECONSTRUCTING A SEMILINEAR TERM FROM INPUT SOURCES	88
5.1	Introduction	88
5.2	Newton method	89
5.3	Quasi-Newton method	91

6. CONCLUSION	93
REFERENCES	95

LIST OF FIGURES

FIGURE	Page
1.1 Decay rates comparison between Gaussian and anomalous diffusion .	18
3.1 Example 3.2.1 Numerical $f(u)$ and exact $f(u)$	65
3.2 Example 3.2.2 Numerical $f(u)$ and exact $f(u)$	66
3.3 The role of α	66
4.1 Example 4.3.1 Exact f and numerical f with different first guesses .	84
4.2 Example 4.3.2 Numerical f and exact f	85
5.1 Example 5.2.1 Exact Q and numerical Q	91
5.2 Example 5.3.1 Exact Q and numerical Q	92

LIST OF TABLES

TABLE	Page
4.1 Relative errors between the correct coefficients and the approximated	87

1. INTRODUCTION

1.1 Basic spaces

In this section, we present the definitions for Lebesgue integrable spaces, including the classical Sobolev spaces, as well as for continuous, absolutely continuous, and Hölder continuous function spaces.

Let $x = \{x_1, x_2, \dots, x_n\} \in \mathbb{R}^n$, where \mathbb{R}^n is the n -dimensional real vector space. Then for real number $p > 1$, the l^p norm of x is defined by

$$\|x\|_p = \left(\sum_{i=1}^n |x_i|^p \right)^{1/p}. \quad (1.1)$$

Let $\Omega = [a, b]$ ($-\infty \leq a < b \leq \infty$) be a finite or infinite interval of the real axis $\mathbb{R} = (-\infty, \infty)$. We use $L^p(a, b)$ ($1 \leq p \leq \infty$) to denote the set of those Lebesgue complex-valued measurable functions f on Ω for which $\|f\|_p < \infty$ where

$$\begin{cases} \|f\|_p = \left(\int_a^b |f(t)|^p dt \right)^{1/p}, & 1 \leq p < \infty \\ \|f\|_\infty = \operatorname{ess\,sup}_{a \leq x \leq b} |f(x)|, & p = \infty, \end{cases} \quad (1.2)$$

where $\operatorname{ess\,sup} |f(x)|$ is the essential maximum of the function $f(x)$.

Let $[a, b]$ be a finite interval and define $AC[a, b]$ to be the space of functions f that are absolutely continuous on $[a, b]$. It is known that $AC[a, b]$ is equivalent to the space of primitives of Lebesgue summable functions([24]):

$$f(x) \in AC[a, b] \Leftrightarrow f(x) = c + \int_a^x \psi(t) dt, \quad \psi(t) \in L(a, b), \quad (1.3)$$

so an absolutely continuous function $f(x)$ has a summable derivative $f'(x) = \psi(x)$

almost everywhere on $[a, b]$.

For $n \in \mathbb{N} = \{1, 2, 3, \dots\}$, we denote by $AC^n[a, b]$ the space of complex-valued functions $f(x)$ that have continuous derivatives up to order $n - 1$ on $[a, b]$ such that $f^{(n-1)}(x) \in AC[a, b]$:

$$AC^n[a, b] = \{f : [a, b] \rightarrow \mathbb{C} \quad \text{and} \quad f^{(n-1)}(x) \in AC[a, b]\}, \quad (1.4)$$

where \mathbb{C} is the set of complex numbers.

Let $\Omega = [a, b] (-\infty \leq a < b \leq \infty)$ and $m \in \mathbb{N}_0 = \{0, 1, 2, \dots, \}$. We denote by $C^m(\Omega)$ a space of functions f that are n times continuously differentiable on Ω with the norm

$$\|f\|_{C^n} = \sum_{k=0}^n \|f^{(k)}\|_C = \sum_{k=0}^n \max_{x \in \Omega} |f^{(k)}|, \quad n \in \mathbb{N}_0. \quad (1.5)$$

In particular, for $n = 0$, $C^0(\Omega) \equiv C(\Omega)$ is the space of continuous function f on Ω with the norm $\|f\|_\infty = \max_{x \in \Omega} |f(x)|$.

$C_C^\infty(\Omega)$ is the space of functions that are infinite differentiable and have compact support in Ω , meaning that the support set of function f defined by $\text{supp}(f) = \{x \in \Omega, f(x) \neq 0\}$ is a compact subset in Ω .

Let Ω be an open subset of some Euclidean space and $n \geq 0$ an integer. We denote by $C^{n,\gamma}(\Omega)$ a space of functions f that are n times continuously differentiable on Ω such that the n -th partial derivatives are Hölder continuous with exponent γ , where $0 < \gamma \leq 1$. Hölder continuous means that the Hölder coefficient

$$|f|_{C^{0,\gamma}} = \sup_{x,y \in \Omega, x \neq y} \frac{|f(x) - f(y)|}{|x - y|^\gamma} \quad (1.6)$$

is finite. We have the important compact embedding result for Hölder spaces([24]),

Theorem 1.1.1 *If Ω is defined as above and let $0 < \alpha < \beta \leq 1$ be two Hölder exponents. Then, we have the inclusion of the corresponding Hölder spaces: $C^{0,\beta}(\Omega) \rightarrow C^{0,\alpha}(\Omega)$, with $\|f\|_{C^{0,\alpha}(\Omega)} \leq \text{diam}(\Omega)^{\beta-\alpha} \|f\|_{C^{0,\beta}(\Omega)}$, where $\text{diam}(\Omega)$ is the diameter of Ω defined as the largest distance between two points in Ω .*

For every function $f \in C^k(\Omega)$ and $\psi \in C_C^\infty(\Omega)$, we have

$$\int_{\Omega} f D^\alpha \psi dx = (-1)^{|\alpha|} \int_{\Omega} \psi D^\alpha f dx,$$

where α is a multi-index of order $|\alpha| = k$ and Ω is an open subset in \mathbb{R}^n . The notation $D^\alpha f$ means

$$D^\alpha f = \frac{\partial^{|\alpha|} f}{\partial x_1^{\alpha_1} \dots \partial x_n^{\alpha_n}}.$$

If there exists a locally integrable function g , such that

$$\int_{\Omega} f D^\alpha \psi dx = (-1)^{|\alpha|} \int_{\Omega} \psi g dx, \quad \psi \in C_C^\infty(\Omega), \quad (1.7)$$

then we call g is the weak α -th partial derivative of f .

The Sobolev space $H^{k,p}(\Omega)$ is defined to be the set of all functions $f \in L^p(\Omega)$ such that for every multi-index α with $|\alpha| \leq k$, the weak partial derivative $D^\alpha f$ belongs to $L^p(\Omega)$, i.e.

$$H^{k,p}(\Omega) = \{f \in L^p(\Omega) : D^\alpha f \in L^p(\Omega), \forall |\alpha| \leq k.\} \quad (1.8)$$

The norm is defined by

$$\|f\|_{H^{k,p}(\Omega)} = \begin{cases} \left(\sum_{|\alpha| \leq k} \|D^\alpha f\|_{L^p(\Omega)}^p \right)^{1/p}, & 1 \leq p < \infty, \\ \max_{|\alpha| \leq k} \|D^\alpha f\|_{L^\infty(\Omega)}, & p = \infty, \end{cases} \quad (1.9)$$

And $H_0^{k,p}(\Omega)$ is defined as $H_0^{k,p}(\Omega) = \{f \in H^{k,p}(\Omega) \text{ and } \mathbf{T}f = 0, \}$ where \mathbf{T} is the trace mapping. For example, from Sobolev space $H^{1,p}(\Omega)$ to $L^p(\partial\Omega)$, there exists a trace mapping \mathbf{T} such that for any function $u \in H^{1,p}(\Omega)$, we have $\|\mathbf{T}u\|_{L^p(\partial\Omega)} \leq C\|u\|_{H^{1,p}(\Omega)}$, where C is a constant.

If $p = 2$, then we usually simplify the notation to $H^k(\Omega)$ and $H_0^k(\Omega)$ respectively.

1.2 Fixed point theory

For nonlinear partial differential equations or linear partial differential equations with nonlinear terms, the iteration scheme is a general technique to apply. Here we list one theoretical result that will be used for our inverse problems.

Definition 1.2.1 ([3]) *Given a linear space X over the real or the complex field, then $\|\cdot\|$ is called a norm if it satisfies the following properties:*

- $\|x\| = 0$ if and only if $x = 0$,
- $\|\lambda x\| = |\lambda|\|x\|$ for any scalar λ , and
- $\|x + y\| \leq \|x\| + \|y\|$.

A linear space X with a norm defined on it is called a *normed space*. In a normed space X , the *distance* between any two points x, y is defined by $\|x - y\|$.

A sequence $\{x_n\}$ is called a *Cauchy sequence* if $\|x_m - x_n\| \rightarrow 0$ as $m, n \rightarrow \infty$. If every Cauchy sequence in X is a convergent sequence, then we say that X is a *complete space*. A complete normed space is called a *Banach space*.

Definition 1.2.2 Let \mathbf{T} be a mapping defined on a set S of a Banach space X and suppose that \mathbf{T} maps S to itself, i.e., $\mathbf{T}x \in S$ if $x \in S$. Then \mathbf{T} is called a contraction if there exists a positive number $\lambda < 1$ such that

$$\|\mathbf{T}x - \mathbf{T}y\| \leq \lambda\|x - y\|,$$

for all $x, y \in S$.

We have the following result for contraction maps([26]).

Theorem 1.2.1 Let \mathbf{T} be a mapping that maps a closed set S into itself, and assume that \mathbf{T} is a contraction in S . Then there exists a unique point $y \in S$ such that $\mathbf{T}y = y$.

Proof Take any $x_0 \in S$ and define successively $x_{n+1} = \mathbf{T}x_n$ for $n = 0, 1, \dots$.

Since \mathbf{T} maps S to itself, all the x_n defined as above belong to S . We further have

$$\|x_{n+1} - x_n\| = \|\mathbf{T}x_n - \mathbf{T}x_{n-1}\| \leq \lambda\|x_n - x_{n-1}\| \leq \dots \leq \lambda^n\|x_1 - x_0\|.$$

Hence,

$$\begin{aligned} \|x_{n+m} - x_n\| &= \left\| \sum_{i=1}^m (x_{n+i} - x_{n+i-1}) \right\| \leq \sum_{i=1}^m \|(x_{n+i} - x_{n+i-1})\| \\ &\leq \left(\sum_{i=1}^m \lambda^{n+i-1} \right) \|x_1 - x_0\| \leq \frac{\lambda^n}{1 - \lambda} \|x_1 - x_0\|. \end{aligned}$$

and $\lim_{n \rightarrow \infty} \frac{\lambda^n}{1 - \lambda} \|x_1 - x_0\| = 0$ since $\lambda < 1$. It follows that $\{x_n\}$ is a Cauchy sequence. Thus it converges to some point $y \in S$. Because S is a closed set in X , $y \in S$. So that

$$\|\mathbf{T}y - y\| = \|\mathbf{T}y - \mathbf{T}x_n + x_{n+1} - y\| \leq \lambda\|y - x_n\| + \|x_{n+1} - y\| \rightarrow 0$$

as $n \rightarrow \infty$, i.e., $\mathbf{T}y = y$.

To prove uniqueness, suppose \bar{y} is another fixed point. Then

$$\|\bar{y} - y\| = \|\mathbf{T}\bar{y} - \mathbf{T}y\| \leq \lambda\|\bar{y} - y\| \leq \cdots \leq \lambda^n\|\bar{y} - y\| \rightarrow 0$$

as $n \rightarrow \infty$, i.e., $\bar{y} = y$. ■

1.3 Volterra equation of the second kind

The Volterra equation of second kind will be used for further discussions in Section 3 and Section 4.

Definition 1.3.1 *For the unknown function f , the given kernel k and the data function g , the Volterra integral equations of the second kind is defined by*

$$f(x) = \int_0^x k(x, t)f(t)dt + g(x), \quad x \in [0, a], \quad (1.10)$$

where $a \in \mathbb{R}$.

We have the following result for the Volterra equations of the second kind ([31]).

Theorem 1.3.1 *If $k(x, t)$ is continuous for $0 \leq t \leq x \leq a$ and $g(x)$ is continuous for $0 \leq x \leq a$, then the equation (1.10) has a unique continuous solution f for $0 \leq x \leq a$.*

The proof is followed by the fixed point theory. See [31].

1.4 Classical diffusion equations

The classical heat equation $u_t(x, t) - \Delta u(x, t) = 0$, $x \in \mathbb{R}^N, t > 0$, where

$$u_t = \frac{\partial u}{\partial t}, \quad \Delta u = \sum_{i=1}^N u_{x_i x_i} = \frac{\partial^2 u}{\partial x_i^2},$$

was first studied by Joseph Fourier in the early 19th century([25]).

1.4.1 Derivation

The diffusion equation can be derived from the continuity equation, which states that a change in density in any part of the system is due to inflow and outflow of material into and out of that part of the system. Effectively, no material is created or destroyed: $\frac{\partial u}{\partial t} + \nabla \cdot \mathbf{j} = 0$, where \mathbf{j} is the flux and $\nabla \cdot$ is the gradient operator, which is defined by $\nabla \cdot u = \sum_{i=1}^N \frac{\partial u}{\partial x_i}$.

When we combine this with Fick's first law, which assumes that the flux of the diffusing material in any part of the system is proportional to the local density gradient:

$$\mathbf{j} = -D\nabla u(\mathbf{r}, t), \quad (1.11)$$

where $D = D(\mathbf{r}, t, u)$ is the diffusion coefficient, we obtain the classical diffusion equation

$$u_t - \nabla \cdot (D\nabla u(\mathbf{r}, t)) = 0. \quad (1.12)$$

1.4.2 Fundamental solutions

Without loss of generality, we can assume $D = 1$ in (1.12). We also only consider the one-dimensional case and so obtain

$$u_t - u_{xx} = 0, \quad -\infty < x < \infty, t > 0, \quad (1.13)$$

combined with the initial condition $u(x, 0) = f(x)$, $-\infty < x < \infty$, where f is a known function. This can be solved by a variety of means, for example, by the Fourier or Laplace transform method. Here we use Fourier transforms.

Let

$$\hat{u}(s, t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} u(\xi, t) \exp(-is\xi) d\xi,$$

then,

$$-s^2 \hat{u}(s, t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} u_{xx}(x, t) \exp(-isx) dx,$$

and we can rewrite (1.13) to the initial-value problem

$$\begin{cases} \hat{u}_t = -s^2 \hat{u}, & t > 0, \\ \hat{u}(s, 0) = \hat{f}(s). \end{cases}$$

Solving the above equation, we obtain $\hat{u}(s, t) = \hat{f}(s) \exp(-s^2 t)$ and now applying the inverse Fourier transform and using the identity

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} \exp(is(x - \xi) - s^2 t) ds = \frac{1}{\sqrt{4\pi t}} \exp\left(-\frac{x^2}{4t}\right),$$

we get the solution for problem (1.13) as follows,

$$u(x, t) = \int_{-\infty}^{\infty} K(x - \xi, t) f(\xi) d\xi, \quad t > 0, \quad (1.14)$$

where

$$K(x, t) = \frac{1}{\sqrt{4\pi t}} \exp\left(-\frac{x^2}{4t}\right) \quad (1.15)$$

is the *fundamental solution*.

1.4.3 Existence and uniqueness

We have the following basic result which is taken from Theorem 3.5.1 and 3.6.1 in [7].

Theorem 1.4.1 *For all piecewise-continuous functions f that satisfy*

$$|f(x)| \leq C_1 \exp(C_2|x|^{1+\gamma}), 0 \leq \gamma < 1,$$

where C_1 and C_2 are positive constants, $u(x, t)$ defined by (1.14) is a solution for problem (1.13). For all piecewise-continuous function f that are asymptotic to $C_1 \exp(C_2x^2)$ at $|x| = \infty$, u is defined only for $0 < t < 1/(4C_2)$ and satisfied the initial-value problem

$$\begin{cases} u_t - u_{xx} = 0, & -\infty < x < \infty, 0 < t < 1/(4C_2), \\ u(x, 0) = f(x), & -\infty < x < \infty \end{cases}$$

Moreover, this solution is unique within the class of solutions v of the initial-value problem that admit a finite number of bounded discontinuities at $t = 0$ and that satisfy a growth condition of the form $|v(x, t)| \leq C_3 \exp(C_4x^2)$, where C_3 and C_4 are positive constants.

1.4.4 Regularity

For (1.13), we have the following smoothing properties([20], Theorem 8 in Section 2.3).

Theorem 1.4.2 *Suppose $u(x, t)$, where $u(\cdot, t) \in C^2(U), U \in \mathbb{R}^N$ and $u(x, \cdot) \in C^1([0, T])$ solves the initial value problem (1.13) , then $u(x, t) \in C^\infty(U \times [0, T])$.*

1.4.5 Maximum principle

Let us extend our classical heat operator $(\frac{d}{dt} - \Delta)$ to (L) , where L is the general parabolic operator defined as

$$Lu = \sum_{i,j=1}^N a_{ij}(x,t) \frac{\partial^2 u}{\partial x_i \partial x_j} + \sum_{i=1}^N b_i(x,t) \frac{\partial u}{\partial x_i} + c(x,t)u - \frac{\partial u}{\partial t} \quad (1.16)$$

in D , where $D \in \mathbb{R}^{N+1}$. We have the following assumptions on L .

- L is parabolic in D , i.e., for every $(x,t) \in D$ and any vector $\xi \neq 0$, $\sum a_{ij}\xi_i\xi_j > 0$;
- the coefficients of L are continuous functions in D ;
- $c(x,t) \leq 0$ in D .

Then we have the following strong maximum principle ([26], Theorem 1 in Section 2).

Theorem 1.4.3 *Let L be defined as (1.16) with these assumptions, then if $Lu \geq 0$ ($Lu \leq 0$) and u has a positive maximum (negative minimum) in D which is a point $P^0(x^0, t^0)$ inside D , then $u(P) = u(P^0)$ for all $P \in S(P^0)$, where $S(P^0)$ means the set of all points Q in D that can be connected to P^0 by a continuous curve in D along which the t -coordinate is nondecreasing to P^0 .*

1.5 Fractional diffusion equations; preliminaries

From the viewpoint of statistical physics, 'normal diffusion' modeled by (1.12) is based on Brownian motion of the particles. The spatial probability density function, evolving in time, which governs the Brownian motion, is a Gaussian distribution whose variance is proportional to the first power of time. In contrast, over the last few

decades several experiments have found "anomalous diffusion" that is characterized by the property that its variance behaves like a non-integer power of time.

1.5.1 Soil pollution

In [42], the authors studied a problem in soil pollution, namely to determine the diffusion of contaminants underground. The size of the area of interest is a few kilometers, but one can only obtain data over the scale of meter lengths. From the obtained diffusion data we can find that there is big difference between the actual diffusion profile and the theoretical one predicted by conventional diffusion equation, which was pointed out by Adams and Gelhar([2]).

1.5.2 Lévy flights

Ordinary diffusion is an important process described by a Gaussian distribution. In one dimension, the probability density $P(x, t)$ of a particle, initially($t = 0$) at $x = 0$, being at x at time t is $P(x, t) = (4\pi t)^{-1/2} \exp(-x^2/4t)$. A main feature of this process is the linear relation between the mean square displacement and time, namely $\langle x^2 \rangle = 2t$. In anomalous diffusion, one might find $\langle x^2 \rangle \propto t^\gamma, \gamma \neq 1$ or else $\langle x^2 \rangle$ might be a divergent integral for $t \neq 0$. The latter process is called Lévy flights. In [9], the author proposed the generalized form of (1.11), where he replaced the ∇u with α -th order($1 < \alpha \leq 2$) Riemann-Liouville fractional derivative, (whose definition we shall meet shortly) and by doing so obtained a fractional order diffusion equation.

Then he rewrote this fractional diffusion equation in an anisotropic medium, in which case it generates the asymmetric Levy statistics instead of the normal Gaussian distribution. It describes so-called 'Lévy flight' very well.

1.5.3 Derivation of fractional diffusion equations

One of the most popular statistical models of anomalous diffusion is a continuous time random walk model that incorporates memory effects and under some realistic assumptions leads to a fractional diffusion equation (see e.g. [2,6,9,27,39,43,54,61] for derivation of the fractional diffusion equations and their applications). For example, in ([39]), the authors showed step by step how to obtain the fractional diffusion equation by the continuous time's random walk model(Equation (34) in [39]).

1.6 Fractional calculus

While the interest in fractional equations for modeling of diffusion is recent, the subject of fractional calculus is not. The concept of fractional calculus is popularly believed to have stemmed from a question raised in the year 1695 by L'Hopital to Leibniz that sought the meaning of Leibniz's notation $\frac{d^n y}{dx^n}$ for the derivative of order n when $n = 1/2$. In his reply, dated 30 September 1695, Leibniz wrote to L'Hopital as follows: "... This is an apparent paradox from which, one day, useful consequences will be drawn. ...". Subsequent mention of fractional derivatives was made by Euler in 1730, Lagrange in 1772, Laplace in 1812, Lacroix in 1819, Fourier in 1822, Abel in 1823, Liouville in 1832, Riemann in 1847, Holmgren in 1865, Grünwald in 1867, Letnikov in 1868, Sonin in 1869, Laurent in 1884, Krug in 1890, Weyl in 1917 and Dzherbashyan in 1960. In fact, in Lacroix's 700-page textbook [32], he devoted two pages (pp. 409-410) to the following result.

First, he pointed out that

$$\frac{d^m}{dx^m} x^n = \frac{n!}{(n-m)!} x^{n-m}, \quad n \in \mathbb{N}, m \in \mathbb{N}_0.$$

Since $n! = \Gamma(n+1)$ and $(n-m)! = \Gamma(n-m+1)$, the above equation can be written

in terms of

$$\frac{d^m}{dx^m} x^n = \frac{\Gamma(n+1)}{\Gamma(n-m+1)} x^{n-m},$$

then if we set $m = \frac{1}{2}$ and $n = 1$,

$$\frac{d^{1/2}}{dx^{1/2}} x = \frac{\Gamma(2)}{\Gamma(3/2)} x^{1/2} = \frac{2\sqrt{x}}{\sqrt{\pi}}.$$

Among these mathematicians, Abel is regarded as the first person to apply fractional integrals. In [1], he studied the solution of the tautochrone (isochrone) problem involving the fractional integral $\int_0^t (t-s)^{-\frac{1}{2}} f(s) ds = C$, where C is a constant with respect to t . He showed the solution is exactly the following half-order Riemann-Liouville fractional derivative of C ,

$$f(t) = \frac{1}{\Gamma(1/2)} \left(\frac{d}{dt}\right)^{1/2} \int_0^t \frac{C}{(t-s)^{1/2}} ds = \frac{C}{\Gamma(1/2)\sqrt{t}}.$$

The first work devoted exclusively to the subject of fractional calculus is the book by Oldham and Spanier([44]) published in 1974. But before that, mathematicians like Dzhrbashyan had done much work on fractional calculus, such as many papers (for example, [15,16]) and one book ([14]), which were all written in Russian. Some of the most recent works on the subject of fractional calculus include the book of Dzhrbashyan([17]) in 1993, Miller([40]) in 1993 and Podlubny([50]) published in 1999, which deal principally with fractional differential equations. Currently, there exist at least two international journals that are devoted almost entirely to the subject of fractional calculus: (i) Journal of Fractional Calculus and (ii) Fractional Calculus and Applied Analysis.

1.7 Mittag-Leffler function

In these two sections, we will talk about two basic functions that are substantial to fractional diffusion equations.

The classical Mittag-Leffler function is first introduced by Mittag-Leffler in [41] and is a special case ($\beta = 1$) of the following definition of the Mittag-Leffler function,

$$E_{\alpha,\beta}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + \beta)}, \quad (1.17)$$

where $z \in \mathbb{C}$, $\alpha, \beta \in \mathbb{R}$. It is an entire function in z with order $\frac{1}{\alpha}$ and type one. The Mittag-Leffler function has close connections with some well-known functions,

$$\begin{aligned} E_{1,1}(z) &= \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(k+1)} = \sum_{k=0}^{\infty} \frac{z^{k+1}}{k!} = e^z, \\ E_{1,2}(z) &= \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(k+2)} = \frac{1}{z} \sum_{k=0}^{\infty} \frac{z^k}{k+2} = \frac{e^z - 1}{z}, \\ E_{2,2}(z) &= \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(2k+2)} = \sum_{k=0}^{\infty} \frac{z^k}{(2k+1)!} = \frac{\sinh(\sqrt{z})}{\sqrt{z}}. \end{aligned}$$

The Mittag-Leffler function has the integral representation

$$E_{\alpha,\beta}(z) = \frac{1}{2\pi} \int_{\mathcal{C}} \frac{t^{\alpha-\beta} e^t}{t^\alpha - z} dt, \quad (1.18)$$

where \mathcal{C} is a contour that starts and ends at $-\infty$ and encircles the circular disk $|t| \leq |z|^{1/\alpha}$ in the positive sense: $|\arg(t)| \leq \pi$ on \mathcal{C} . This representation is useful to prove the asymptotic behavior of Mittag-Leffler functions.

1.7.1 Derivatives

For any integer m , we have the following derivative formula,

$$\left(\frac{d}{dt}\right)^m(t^{\beta-1}E_{\alpha,\beta}(t^\alpha)) = t^{\beta-m-1}E_{\alpha,\beta-m}(t^\alpha). \quad (1.19)$$

Take $\alpha = \frac{m}{n}$, where m, n are integers, then we get

$$\left(\frac{d}{dt}\right)^m(t^{\beta-1}E_{m/n,\beta}(t^\alpha)) = t^{\beta-1}E_{m/n,\beta-m}(t^{m/n}) + t^{\beta-1} \sum_{k=1}^n \frac{t^{-\frac{m}{n}k}}{\Gamma(\beta - \frac{m}{m}k)}. \quad (1.20)$$

Then set $n = 1$, $\beta \in \mathbb{N}$ to get

$$\left(\frac{d}{dt}\right)^m(t^{\beta-1}E_{m,\beta}(t^m)) = t^{\beta-1}E_{m,\beta}(t^m), \quad (1.21)$$

where we have applied $\frac{1}{\Gamma(-\nu)} = 0$, $\nu \in \mathbb{N}$.

1.7.2 Laplace transform

We have

$$\int_0^\infty e^{-pt}t^{\alpha k + \beta - 1}E_{\alpha,\beta}^{(k)}(\pm at^\alpha)dt = \frac{k!p^{\alpha-\beta}}{(p^\alpha \mp a)^{k+1}}, \quad \operatorname{Re}(p) > |a|^{1/\alpha},$$

where $\operatorname{Re}(p)$ is the real part of complex number p .

The particular case of the above Laplace pair is that when $\alpha = \beta = \frac{1}{2}$,

$$\int_0^\infty e^{-pt}t^{\frac{k-1}{2}}E_{1/2,1/2}^{(k)}(\pm a\sqrt{t})dt = \frac{k!}{(\sqrt{p} \mp a)^{k+1}}, \quad \operatorname{Re}(p) > a^2.$$

1.7.3 Asymptotic behavior

The asymptotic behavior of Mittag-Leffler functions are different for $\alpha < 2$, $\alpha = 2$ and $\alpha > 2$ ([50],Section 1.2.7).

Theorem 1.7.1 *If $0 < \alpha < 2$, β is an arbitrary complex number and μ is an arbitrary real number such that*

$$\frac{\pi\alpha}{2} < \mu < \min\{\pi, \pi\alpha\}, \quad (1.22)$$

then for an arbitrary integer $p \geq 1$, the following expansions hold,

$$E_{\alpha,\beta}(z) = \frac{1}{\alpha} z^{(1-\beta)/\alpha} \exp(z^{1/\alpha}) - \sum_{k=1}^p \frac{z^{-k}}{\Gamma(\beta - \alpha k)} + O(|z|^{-1-p}), \quad |z| \rightarrow \infty, |\arg(z)| \leq \mu. \quad (1.23)$$

and

$$E_{\alpha,\beta}(z) = - \sum_{k=1}^p \frac{z^{-k}}{\Gamma(\beta - \alpha k)} + O(|z|^{-1-p}), \quad |z| \rightarrow \infty, \mu \leq |\arg(z)| \leq \pi, \quad (1.24)$$

where $\arg(z)$ is the argument of complex number z .

Theorem 1.7.2 *If $\alpha < 2$, β is an arbitrary complex number and μ is an arbitrary real number such that $\frac{\pi\alpha}{2} < \mu < \min\{\pi, \pi\alpha\}$, and C_1, C_2 are real constants, then*

$$|E_{\alpha,\beta}(z)| \leq C_1(1+|z|)^{(1-\beta)/\alpha} \exp(\operatorname{Re}(z^{1/\alpha})) + \frac{C_2}{1+|z|}, \quad |\arg(z)| \leq \mu, |z| \geq 0. \quad (1.25)$$

$$|E_{\alpha,\beta}(z)| \leq \frac{C}{1+|z|}, \quad \mu \leq |\arg(z)| \leq \pi, |z| \geq 0. \quad (1.26)$$

Theorem 1.7.3 *If $\alpha \geq 2$, β is an arbitrary complex number, then for arbitrary*

integer number $p > 1$, the following asymptotic formula holds:

$$E_{\alpha,\beta}(z) = \frac{1}{\alpha} \sum_n (z^{1/\alpha} e^{(2\pi ni/\alpha)})^{1-\beta} \exp\{\exp(\frac{2\pi ni}{\alpha}) z^{1/\alpha}\} - \sum_{k=1}^p \frac{z^{-k}}{\Gamma(\beta - \alpha k)} + O(|z|^{-1-p}), \quad (1.27)$$

where the sum is taken for integer n satisfying the condition $|\arg(z) + 2\pi n| \leq \frac{\pi\alpha}{2}$.

$E_{\alpha,1}(-\pi^2 t^\alpha)$ is the fundamental solution for the following problem

$$\begin{cases} \partial_t^\alpha u - u_{xx} = 0, & 0 < x < 1, \quad t > 0, \\ u(x, 0) = \sin(\pi x), & 0 < x < 1, \\ u(0, t) = u(1, t) = 0, & t > 0 \end{cases} \quad (1.28)$$

In Figure 1.1, we show the decay rate of Mittag-Leffler function $E_{\alpha,1}(-\pi^2 t^\alpha)$ when $\alpha = \{1, 0.75, 0.5, 0.25\}$. We can see that in a short time interval, it decays much faster than normal diffusion, but for large time values, it decays more slowly. We also notice that the smaller α is, the slower it decays.

1.8 Wright functions

We then introduce a special function, the so-called M function of the Wright type, whose general properties are discussed in [22, 38].

The Wright function is defined as:

$$W_{\alpha,\beta}(z) = \sum_{k=0}^{\infty} \frac{z^k}{k! \Gamma(\alpha k + \beta)}, \quad (1.29)$$

which is also an entire function in z .

The special case $\alpha = -\mu, \beta = 1 - \mu, \mu \in (0, 1)$ of W is denoted by $M_\mu(z)$,

$$M_\mu(z) := W_{-\mu, 1-\mu}(-z) \quad (1.30)$$

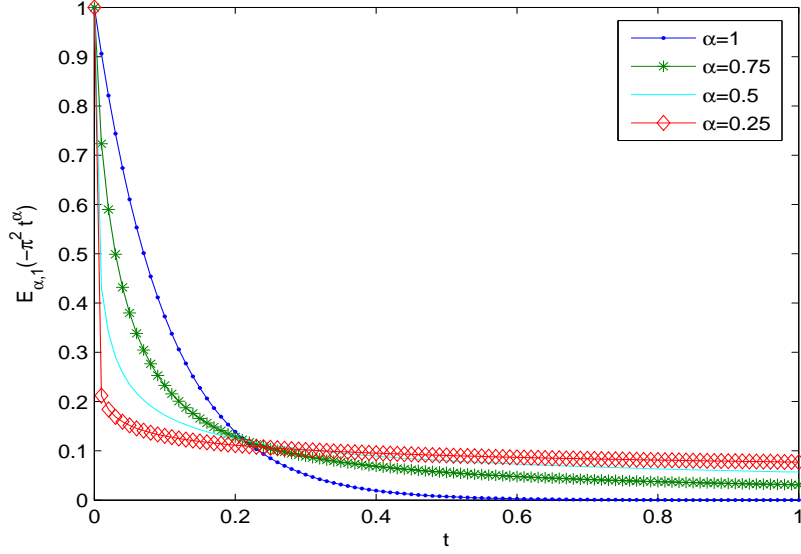


Figure 1.1: Decay rates comparison between Gaussian and anomalous diffusion

and is often referred to as the Mainardi function. We have

$$M_\mu(z) := \frac{1}{\pi} \sum_{k=1}^{\infty} \frac{(-z)^{k-1}}{(k-1)!} \Gamma(\mu k) \sin(\pi \mu k), \quad z \in \mathbb{C}, \quad (1.31)$$

which will be used to construct fundamental solutions for fractional diffusion equations. $M_\mu(z)$ is an entire function of order $\rho = 1/(1-\mu)$ and for $\mu = 1/2$ and $\mu = 1/3$ it becomes the familiar Gaussian and Airy functions:

$$M_{1/2}(z) = \frac{1}{\sqrt{\pi}} \exp(-z^2/4), \quad M_{1/3}(z) = 3^{2/3} \text{Ai}(z/3^{1/3}).$$

1.8.1 Laplace transform

We have the following Laplace transforms for Wright function,

$$\mathcal{L}\{W_{\alpha,\beta}(t); s\} = \frac{1}{s} E_{\alpha,\beta}(1/s), \quad \alpha > -1, \text{Re}(s) > 0 \quad (1.32)$$

For function M_μ ,

$$\begin{cases} \mathcal{L}\{M_\mu(t/c); s\} = cE_{\alpha,1}(-cs), & \operatorname{Re}(s) > 0, \\ \mathcal{L}\{t^{-\mu}M_\mu(ct^{-\mu}); s\} = s^{\mu-1}\exp(-cs^\mu), & \operatorname{Re}(s) > 0, \\ \mathcal{L}\{c\mu t^{-\mu-1}M_\mu(ct^{-\mu}); s\} = \exp(-cs^\mu), & \operatorname{Re}(s) > 0. \end{cases} \quad (1.33)$$

1.8.2 Asymptotic behavior

When $|z| \rightarrow \infty$, the Wright function has the following asymptotic behavior.

$$W_{\alpha,\beta}(z) = a_0(\alpha z)^{(1-\beta)/(1+\alpha)} \exp\left[\left(1 + \frac{1}{\alpha}\right)(\alpha z)^{1/(1+\alpha)}\right] \left[1 + O\left(\left(\frac{1}{z}\right)^{1/(1+\alpha)}\right)\right], \quad z \in \mathbb{C}, \quad (1.34)$$

where $a_0 = [2\pi(\alpha + 1)]^{-1/2}$ and $|\arg(z)| \leq \pi - \varepsilon$ ($0 < \varepsilon < \pi$).

For the function M_μ , there is

$$M_\mu(x) \sim Ax^a \exp(-bx^c), \quad x \rightarrow \infty \quad (1.35)$$

with

$$A = \left(2\pi(1-\mu)\mu^{\frac{1-2\mu}{1-\mu}}\right)^{-1/2}, \quad a = \frac{2\mu-1}{2-2\mu}, \quad b = (1-\mu)\mu^{\frac{\mu}{1-\mu}}, \quad c = \frac{1}{1-\mu}.$$

From this we see immediately that $M_\mu(x)$ decays faster than the linear exponential order but slower than Gaussian as $x \rightarrow \infty$ when $0 < \mu = \alpha/2 < 1/2$. This property is in line with the alternate diffusion concept as in some situations Gaussian diffusion decays faster than is seen in practice.

2. PRELIMINARIES

2.1 Fractional derivatives

In the literature, several different definitions of the fractional derivatives, including the Caputo, Grünwald-Letnikov, Riemann-Liouville, and Riesz derivatives (see e.g. [30, 50]), were proposed. All of them are related to each other and are defined as non-local operators in contrast to the integer order derivatives that are local operators. In my dissertation, the Riemann-Liouville and Caputo fractional derivatives are employed following a long series of other researches, where fractional differential equations with the Riemann-Liouville derivatives and the Caputo derivatives were introduced as models for different real world processes.

2.1.1 Riemann-Liouville derivative

The left-sided Riemann-Liouville fractional derivative D_{a+}^{α} of order $\alpha \in \mathbb{C}$ is defined by

$$D_{a+}^{\alpha} u(t) = \frac{1}{\Gamma(n - \alpha)} \left(\frac{d}{dt}\right)^n \int_a^t \frac{u(s)}{(t - s)^{\alpha - n + 1}} ds \quad (n - 1 \leq \operatorname{Re}(\alpha) \leq n). \quad (2.1)$$

The right-sided Riemann-Liouville fractional derivative D_{b-}^{α} of order $\alpha \in \mathbb{C}$ is defined by

$$D_{b-}^{\alpha} u(t) = \frac{1}{\Gamma(n - \alpha)} \left(\frac{d}{dt}\right)^n \int_t^b \frac{u(s)}{(t - s)^{\alpha - n + 1}} ds \quad (n - 1 \leq \operatorname{Re}(\alpha) \leq n). \quad (2.2)$$

Hereafter, only the left-sided Riemann-Liouville derivatives will be used, particularly the left-sided Riemann-Liouville derivative from $a = 0$, D_{0+}^{α} .

We have the following existence result for Riemann-Liouville derivatives.

Theorem 2.1.1 (Lemma 2.2 in [30]) Let $u(t) \in AC^n[a, b]$, where $AC^n[a, b]$ is defined as (1.4) in Section 1.1. Then $D_{a+}^\alpha u$ exists almost everywhere for $n-1 < \alpha < n$.

We have the following Laplace transform for Riemann-Liouville derivatives,

Theorem 2.1.2 If $n-1 \leq \alpha \leq n$, $y(x) \in AC^n[0, b]$ for any $b > 0$, where $AC^n[0, b]$ is defined as (1.4), and the estimate $|y(x)| \leq Be^{q_0 x}$ ($x > b > 0$) holds for constants $B > 0$ and $q_0 > 0$, and if $y^{(k)} = 0, k = 0, 1, 2, \dots, n-1$, then the relation

$$\mathcal{L}(D_{0+}^\alpha y; s) = s^\alpha \mathcal{L}(y; s) \quad (2.3)$$

is valid for $\text{Re}(s) > q_0$.

2.1.2 Caputo derivative

The definition of the fractional differentiation of the Riemann-Liouville type (2.1) played an important role in the development of the theory of fractional derivatives and integrals and has many applications in pure mathematics (solution of integer-order differential equations, definitions of new function classes and summation of series). A number of works have appeared, especially in the theory of viscoelasticity and in hereditary solid mechanics, where fractional derivatives are used for a better description of material properties. Mathematical modelling based on enhanced rheological models naturally leads to differential equations of fractional order and to the necessity to formulate the initial conditions for such equations. Applied problems require definitions of fractional derivatives that allows for the use of physically interpretable initial conditions that contain $u(a), u'(a)$, etc. Unfortunately, the Riemann-Liouville approach leads to initial conditions containing its limit values at the lower terminal $t = a$. In spite of the fact that the initial value problem with

such initial conditions can be successfully solved mathematically, there is no known physical interpretation for such conditions.

A solution to this conflict is another type of fractional derivative, the Caputo derivative, which was first proposed by Caputo in [8]. The left-sided Caputo derivative ∂_{a+}^α of order $\alpha \in \mathbb{C}$ is defined by

$$\partial_{a+}^\alpha u(t) = \frac{1}{\Gamma(n-\alpha)} \int_a^t \frac{u^{(n)}(s)}{(t-s)^{\alpha-n+1}} ds \quad (n-1 \leq \operatorname{Re}(\alpha) \leq n). \quad (2.4)$$

The right-sided Caputo derivative ∂_{b-}^α of order α is defined by

$$\partial_{b-}^\alpha u(t) = \frac{1}{\Gamma(n-\alpha)} \int_t^b \frac{u^{(n)}(s)}{(t-s)^{\alpha-n+1}} ds \quad (n-1 \leq \operatorname{Re}(\alpha) \leq n). \quad (2.5)$$

We will only use the left-sided Caputo derivatives in the following parts, especially the one from $a = 0$, ∂_{0+}^α , and denote it with ∂_t^α .

We have the following relation between the Riemann-Liouville derivative and the Caputo derivative which will be used later (see Section 2.4 in [30]).

Lemma 2.1.1

$$D_{a+}^\alpha u(t) = \sum_{k=0}^{n-1} \frac{1}{\Gamma(k+1-\alpha)} \frac{u^{(k)}(a)}{(t-a)^\alpha} + \partial_{a+}^\alpha u(t). \quad (2.6)$$

By the definition of Caputo derivative (2.4), we can perform the following derivation,

$$\begin{aligned} \lim_{\alpha \rightarrow n} \partial_{a+}^\alpha u(t) &= \lim_{\alpha \rightarrow n} \left(\frac{u^{(n)}(a)(t-a)^{n-\alpha}}{\Gamma(n-\alpha+1)} + \frac{1}{\Gamma(n-\alpha+1)} \int_a^t (t-\tau)^{n-\alpha} u^{(n+1)}(\tau) d\tau \right) \\ &= u^{(n)}(a) + \int_a^t u^{(n+1)}(\tau) d\tau = u^{(n)}(t), \end{aligned}$$

i.e., when $\alpha \rightarrow n$, the Caputo derivative $\partial_{a+}^\alpha u(t)$ is exactly the classical derivative.

By similar calculation, we can get the same result for the Riemann-Liouville derivative $D_{a+}^\alpha u(t)$, that is, $D_{a+}^n u(t) = u^{(n)}(t)$.

2.1.3 Differences between two derivatives

Take $u(t) = C$, where C is a constant in the definitions (2.1) and (2.4), then we can easily get the first difference. Since the Caputo derivative calculates the classical derivative first, and the conventional derivative of any constant is zero, we obtain, $\partial_{a+}^\alpha C = 0$. Conversely, the Riemann-Liouville derivative calculates the integral first, so $D_{a+}^\alpha C \neq 0$.

In fact, we have that

$$D_{a+}^\alpha C = \frac{Ct^{-\alpha}}{\Gamma(1-\alpha)}. \quad (2.7)$$

Theoretically, this difference leads to different requirements of function spaces for each definition. As shown in the Lemma 2.1.1, we need $u \in AC^n[a, b]$ to ensure $D_{a+}^\alpha u$ is well-defined, but for $\partial_{a+}^\alpha u$, we need some larger function space.

There is also another difference between the Riemann-Liouville derivatives and the Caputo derivatives that we would like to mention here and is important for applications. That is, for the Riemann-Liouville derivatives, we have

$$D_{a+}^m (D_{a+}^\alpha u(t)) = D_{a+}^{m+\alpha} u(t), \quad m \in \mathbb{N}, \quad (2.8)$$

And for Caputo derivatives, we have

$$\partial_{a+}^m (\partial_{a+}^\alpha u(t)) = \partial_{a+}^{m+\alpha} u(t), \quad m \in \mathbb{N},$$

But the commutativities of these two derivatives require different conditions.

$$D_{a+}^m(D_{a+}^\alpha u(t)) = D_{a+}^{m+\alpha}u(t) = D_{a+}^\alpha(D_{a+}^m u(t)), \quad m \in \mathbb{N},$$

when $u^{(k)}(a) = 0, k = 0, 1, 2, \dots, m$.

While

$$\partial_{a+}^m(\partial_{a+}^\alpha u(t)) = \partial_{a+}^{m+\alpha}u(t) = \partial_{a+}^\alpha(\partial_{a+}^m u(t)), \quad m \in \mathbb{N},$$

when $u^{(k)}(a) = 0, k = n, n + 1, n + 2, \dots, m$.

2.2 New properties

2.2.1 Composition

In the case of Riemann-Liouville derivatives, we have

$$D_{a+}^\alpha(D_{a+}^\beta u(t)) = D_{a+}^{\alpha+\beta}u(t) - \sum_{j=1}^n (D_{a+}^{\beta-j}u(t))|_{t=a} \frac{(t-a)^{-\alpha-j}}{\Gamma(1-\alpha-j)},$$

where $m - 1 \leq \alpha \leq m, n - 1 \leq \beta \leq n$. Thus in the general case, Riemann-Liouville derivatives do not commute with respect to the index.

2.2.2 Leibniz rule

We have the Riemann-Liouville derivative of $(t - a)^n$ as follows.

$$D_{a+}^\alpha(t - a)^n = \frac{\Gamma(n + 1)}{\Gamma(n + 1 - \alpha)}(t - a)^{n-\alpha}.$$

Take $n = 2, 3$ and $a = 0$, then we have

$$D_{0+}^\alpha t^2 = \frac{2}{\Gamma(3 - \alpha)}t^{2-\alpha}, \quad D_{0+}^\alpha t^3 = \frac{6}{\Gamma(4 - \alpha)}t^{3-\alpha}, \quad D_{0+}^\alpha t^5 = \frac{120}{\Gamma(6 - \alpha)}t^{5-\alpha},$$

so that

$$D_{0+}^{\alpha} t^5 \neq t^3 D_{0+}^{\alpha} t^2 + t^2 D_{0+}^{\alpha} t^3.$$

In fact, we have the following fractional Leibniz rule

$$D_{a+}^{\alpha} (f(t)g(t)) = \sum_{k=0}^n \binom{p}{k} f^{(k)}(t) D_{a+}^{p-k}(g(t)) - R_n^p(t),$$

where $R_n^p(t) = \frac{1}{\Gamma(-p)} \int_a^t (t-\tau)^{-p-1} g(\tau) d\tau \int_{\tau}^t f^{(n+1)}(\xi) (\tau-\xi)^n d\xi$.

The new Leibniz rule will cause significant problems. Some consequences are: the product rule fails, thus the usual integration by parts formula, which in turn impacts many of the other tools commonly used in partial differential equations. This fundamentally changes the analysis, or at least the techniques required to obtain useful results.

2.3 New phenomena

By the definitions of (2.1) and (2.4), both fractional derivative definitions show a radical difference from classical derivatives: they are no longer pointwise operators. As mentioned above, these turn out to have some similarities with the classical case but also some differences. These will generate new phenomena for our research.

2.3.1 Backward problem

The backward problem for classical diffusion equations, which uses the data afterwards to reconstruct the information at earlier time, is notoriously ill-conditioned. One way to look at this is the following. The solution profile at time T is determined only by data on a previous time level $T - \varepsilon$ for any $\varepsilon > 0$, so that the information at previous times $t \ll T$ is rapidly lost. To show it explicitly, we consider the following

problem,

$$\begin{cases} u_t - u_{xx} = 0, & 0 \leq x \leq 1, t > 0, \\ u(0, t) = u(1, t) = 0, & t > 0, \\ u(x, 0) = f(x), & 0 \leq x \leq 1, \end{cases} \quad (2.9)$$

and we want to determine the initial temperature $f(x)$ by giving the temperature profile at time $t = 1$, i.e., $u(x, 1) = g(x)$. Could we use the values of $g(x)$ to determine $f(x)$?

By separation of variables, we can get the direct solution for problem 2.9 as follows

$$u(x, t) = \sum_{n=1}^{\infty} c_n e^{-n^2 \pi^2 t} \sin(n\pi x), \quad (2.10)$$

where $c_n = \frac{1}{\pi} \int_0^1 f(x) \sin(n\pi x) dx$. So that the n -th Fourier coefficients c_n of the function $f(x)$ and those, say d_n of $g(x)$ are related by

$$d_n = e^{-n^2 \pi^2} c_n.$$

Thus $c_n = e^{n^2 \pi^2} d_n$, where $d_n = \frac{1}{\pi} \int_0^1 g(x) \sin(n\pi x) dx$, which means we can recover $f(x)$ uniquely. But suppose we only want to recover the first 5 Fourier modes of f , then $c_5 = e^{25 \pi^2} d_5 \approx e^{250} d_5 \approx 10^{110} d_5$. We would have to be able to measure d_5 to hundreds of figures of accuracy.

However, Yamamoto and Sakamoto have shown that due to the required dependence on *all* previous times for fractional derivatives, all the information from previous time values is retained. In consequence, the backward problem for the fractional diffusion equations, where the time derivative is replaced by one of the fractional derivatives, is only mildly ill-conditioned. The precise statement is

Theorem 2.3.1 (Theorem 4.1 in [53]). Let $T > 0$ be arbitrary fixed. For any given $a_1 \in H^2(\Omega) \cap H_0^1(\Omega)$, there exists a unique weak solution $u \in C([0, T]; L^2(\Omega)) \cap C((0, T]; H^2(\Omega) \cap H_0^1(\Omega))$ to problem (2.9) (u_t is replaced by $\partial_t^\alpha u$) such that $u(\cdot, T) = a_1$. Moreover there exist constants $C_1, C_2 > 0$ such that

$$C_1 \|u(\cdot, 0)\|_{L^2(\Omega)} \leq \|u(\cdot, T)\|_{H^2(\Omega)} \leq C_2 \|u(\cdot, 0)\|_{L^2(\Omega)},$$

where C_1, C_2 are independent of choices of a_1 . $L^2(\Omega), H^2(\Omega), H_0^1(\Omega)$ are defined as in Section 1.1.

2.3.2 Inverse Sturm-Liouville problem

Next, we consider

$$\begin{cases} u_{xx} + q(x)u = \lambda u, & 0 < x < 1, \\ u(0) = u(1) = 0, & t > 0, \end{cases} \quad (2.11)$$

and we wish to solve the inverse problem of recovering the potential $q(x)$ from one or more spectra $\{\lambda_k\}$. It is known that for this problem one spectrum is not sufficient unless some additional information is given. For example, if $q(x)$ is known to be symmetric about the midpoint of the interval or is given on one half of the interval and has to be determined on the other half.

But if we just replace u_{xx} with the α -th order Caputo fractional derivative ∂_t^α ($1 < \alpha < 2$), it was shown in [28](Section 4), one single (Dirichlet) spectrum completely determines the potential $q(x)$ in the fractional Sturm-Liouville problem (2.11).

2.3.3 Numerical mechanism

When the Riemann-Liouville and Caputo fractional derivatives of $u(t)$ are no longer pointwise this has considerable consequences from a numerical computation

standpoint. If we compute the solution at a finite series of steps $\{t_0, t_1, \dots, t_{n-1}, t_n\}$ then in the case of the heat equation (or indeed any parabolic equation) the value of the solution at time step t_N depends only on the value at the previous step t_{N-1} . In the case of fractional derivatives value of the solution at time step t_N depends on all of $\{t_n\}_0^{N-1}$. Thus we must store all solution values at all previous time steps. Of course, these must be suitably weighted as we will see shortly.

New schemes also generate challenges for high-order accuracy algorithms. For a classical diffusion equation, we can easily get second order approximation by the finite difference scheme, while for fractional diffusion equations, the best approximation is only $2 - \alpha$. Thus when α is close to 1, one only obtains approximately first order accuracy.

2.4 Direct solution for fractional diffusion equations

2.4.1 Fundamental solutions

Consider

$$\partial_t^\alpha u - u_{xx} = 0, \quad x \in \mathbb{R}, t > 0, \quad (2.12)$$

combined with the initial and boundary conditions

$$\begin{cases} u(x, 0) = h(x), x \in \mathbb{R}, \\ u(-\infty, t) = 0, t > 0, \\ u(+\infty, t) = 0, t > 0, \end{cases} \quad (2.13)$$

where $h(x)$ is a known function. We can solve this by Laplace Transforms.

We introduce the Green function $K_\alpha(x, t)$ for the initial-boundary-value problem (2.12) and (2.13). It represents the fundamental solution of the problem, i.e. the problem with $h(x) = \delta(x)$ in (2.13), where δ is the Dirac δ -function.

Using standard Laplace transform techniques, the fundamental solution $K_\alpha(x, t)$ for problem (2.12) and (2.13) can be obtained in the form

$$K_\alpha(x, t) = \frac{1}{2}t^{-\alpha/2}W_{-\alpha/2, 1-\alpha/2}(-r), \quad t > 0, x \geq 0, \quad (2.14)$$

where $r = xt^{-\alpha/2}$.

Then the solution for problem (2.12) and (2.13) can be written as

$$u_\alpha(x, t) = \int_{-\infty}^{-\infty} K_\alpha(x - \xi, t)h(\xi)d\xi, \quad (2.15)$$

where $K_\alpha(x, t)$ is the fundamental solution,

$$K_\alpha(x, t) = \frac{1}{2}t^{-\alpha/2}M_{\alpha/2}(|x|/t^{\alpha/2}), \quad x \in \mathbb{R}, t > 0, \quad (2.16)$$

which plays the same role with (1.15) for classical diffusion equations.

Then a representation of the solution to the fractional diffusion equations with initial-boundary conditions in a bounded domain can be constructed via similar techniques with the usual θ function for the heat equation as defined in (1.14). We consider the generalization of θ by θ_α defined as

$$\theta_\alpha(x, t) = \sum_{m=-\infty}^{+\infty} K_\alpha(x + 2m, t), \quad t > 0 \quad (2.17)$$

and we have

Lemma 2.4.1 *The function $\theta_\alpha(x, t)$ is an C^∞ function of $x \in \mathbb{R}$ and C^∞ for $t > 0$. It is also an even function with respect to x .*

Proof Using the notation $r_m = |x + 2m|/t^{\alpha/2}$, $m \in \mathbb{Z}$, the formula (2.17) can be

represented in the form

$$\theta_\alpha(x, t) = \sum_{m=-\infty}^{\infty} \frac{1}{2} t^{-\alpha/2} M_{\alpha/2}(r_m) \quad (2.18)$$

where M is defined in (1.30).

The asymptotic behavior of $M_\mu(r)$ as $r \rightarrow \infty$ is shown in (1.35). Now we apply (1.35) with $\mu = \alpha/2$ and $r = r_m$ to the representation (2.18) of the θ_α -function. For $0 < \alpha < 1$, the value of μ is between 0 and $\frac{1}{2}$ and thus for the constants in (1.35) the inequalities $b > 0$ and $1 < c < 2$ hold true. We then get

$$|\theta_\alpha(x, t)| < \sum_{m=-\infty}^{\infty} \frac{1}{2} t^{-\alpha/2} A r_m^a \exp(-b r_m^c) < C \sum_{m=-\infty}^{\infty} \frac{1}{2} t^{-\alpha/2} A r_m^a \exp(-b r_m),$$

where C is a constant. If the inequality $e^{-b r_m^c} < e^{-b r_m}$ holds for all $t > 0$, then we can simply take $C = 1$. When $r_m < 1$, and t is large, since $r_m = |x + 2m|/t^{\alpha/2}$, we can find an integer M , such that $r_m > 1$ for all $m > M$ and then $e^{-b r_m^c} < e^{-b r_m}$. We can split the series into a finite part with indices $|m| \leq M$ and the remaining terms with $|m| > M$. Since all terms of the series are positive, the finite part can be bounded by a constant times the sum while the remaining terms allow the bound $C = 1$.

Let us denote the function $t^{-\alpha/2} A r_m^a \exp(-b r_m)$ by $u_m(x, t)$. Then for any $t_0 > 0$, $t \geq t_0 > 0$, there is an integer M such that the equality $|r_{m+1}| - |r_m| = \frac{2}{t^{\alpha/2}}$ holds if $m > M$. Restricting m to this range we get

$$\lim_{m \rightarrow \infty} \frac{u_{m+1}}{u_m} = \lim_{m \rightarrow \infty} \left(\frac{|x + 2(m+1)|}{|x + 2m|} \right)^a \exp\left(-\frac{2b}{t^{\alpha/2}}\right) = \exp\left(-\frac{2b}{t^{\alpha/2}}\right) < 1$$

since $b > 0$ and $t \geq t_0 > 0$. Thus the series $\sum_{m=0}^{\infty} u_m(x, t)$ is uniformly convergent

for $x \in \mathbb{R}$ and $t \geq t_0 > 0$. Similarly, there exists an integer N such that for all $m < N$, we have $|r_{m-1}| - |r_m| = \frac{2}{t^{\alpha/2}}$ and

$$\lim_{m \rightarrow -\infty} \frac{u_{m-1}}{u_m} = \lim_{m \rightarrow -\infty} \left(\frac{|x + 2(m-1)|}{|x + 2m|} \right)^a \exp\left(-\frac{2b}{t^{\alpha/2}}\right) = \exp\left(-\frac{2b}{t^{\alpha/2}}\right) < 1,$$

so that the series $\sum_{m=-\infty}^0 u_m(x, t)$ also uniformly converges for $x \in \mathbb{R}$ and $t > 0$. Thus the series for $\theta_\alpha(x, t)$ is uniformly convergent for $x \in \mathbb{R}$ and $t \geq t_0 > 0$, too. Using the same technique, we can show that the series for all partial derivatives of θ_α are also uniformly convergent for $x \in \mathbb{R}$ and $t > 0$ showing that θ_α is $C^\infty(-\infty, \infty)$ in x and $C^\infty(0, \infty)$ in t . ■

2.4.2 Properties of the fundamental solution

In general, the product rule for fractional derivatives fails in the usual sense, so we can expect the same for the integration by parts formula. However, we can show that,

Lemma 2.4.2 *Let $f, g \in AC[a, b]$, where $AC[a, b]$ is defined as (1.4) in Section 1.1. Then the integration by parts formula*

$$\int_0^t D_{0+}^\alpha f(t - \tau)g(\tau)d\tau = \int_0^t f(t - \tau)D_{0+}^\alpha g(\tau)d\tau. \quad (2.19)$$

holds true.

Proof The proof is by direct computation. Using Lemma 2.1.1, the left hand side

of (2.19) can be transformed to the form

$$\begin{aligned}
\int_0^t D_{0+}^\alpha f(t-\tau)g(\tau)d\tau &= \int_0^t \frac{1}{\Gamma(1-\alpha)} \left(\int_0^{t-\tau} \frac{f'(s)}{((t-\tau)-s)^\alpha} ds + \frac{f(0)}{(t-\tau)^\alpha} \right) g(\tau)d\tau \\
&= \frac{1}{\Gamma(1-\alpha)} \int_0^t \int_0^{t-\tau} \frac{f'(s)g(\tau)}{((t-\tau)-s)^\alpha} dsd\tau + \frac{f(0)}{\Gamma(1-\alpha)} \int_0^t \frac{g(\tau)}{(t-\tau)^\alpha} d\tau \\
&=: J_1 + J_2.
\end{aligned}$$

By the change of variables $\mu = t - \tau$ and then $\rho = t - \mu$ and $t - s = \tau$ we get the following chain of equalities:

$$\begin{aligned}
J_1 &= \frac{1}{\Gamma(1-\alpha)} \int_0^t \int_0^\mu \frac{f'(s)g(t-\mu)}{(\mu-s)^\alpha} dsd\mu = \frac{1}{\Gamma(1-\alpha)} \int_0^t \int_s^t \frac{g(t-\mu)}{(\mu-s)^\alpha} d\mu f'(s)ds \\
&= \frac{f(s)}{\Gamma(1-\alpha)} \int_s^t \frac{g(t-\mu)}{(\mu-s)^\alpha} d\mu \Big|_{s=0}^{s=t} - \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{\partial}{\partial s} \left(\int_s^t \frac{g(t-\mu)}{(\mu-s)^\alpha} d\mu \right) f(s)ds \\
&= -\frac{f(0)}{\Gamma(1-\alpha)} \int_0^t \frac{g(t-\mu)}{\mu^\alpha} d\mu + \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{\partial}{\partial s} \left(\int_0^{t-s} \frac{g(\rho)}{(t-s-\rho)^\alpha} d\rho \right) f(s)ds \\
&= -J_2 + \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{\partial}{\partial \tau} \left(\int_0^\tau \frac{g(\rho)}{(\tau-\rho)^\alpha} d\rho \right) f(t-\tau)d\tau \\
&= -J_2 + \int_0^t f(t-\tau)D_{0+}^\alpha g(\tau)d\tau.
\end{aligned}$$

This completes the proof. ■

In the following lemmas, some properties of θ_α we need in further discussions are formulated and proved.

Lemma 2.4.3 *The following formulas hold true for $\theta_\alpha(x, t)$ ($0 < \alpha < 1$):*

$$\theta_\alpha(0, t) = c_0(\alpha)t^{-\alpha/2} + 2 \sum_{m=1}^{\infty} K_\alpha(2m, t) =: c_0(\alpha)t^{-\alpha/2} + H(t), \quad (2.20)$$

$$\theta_\alpha(1, t) = \theta_\alpha(-1, t) =: G(t), \quad (2.21)$$

$$\lim_{x \rightarrow 0^+} \mathcal{L} \left\{ \frac{\partial \theta_\alpha}{\partial x}(x, t); s \right\} = -\frac{1}{2}s^{\alpha-1}, \quad \lim_{x \rightarrow 0^-} \mathcal{L} \left\{ \frac{\partial \theta_\alpha}{\partial x}(x, t); s \right\} = \frac{1}{2}s^{\alpha-1}, \quad (2.22)$$

$$\lim_{x \rightarrow 0^+} \mathcal{L} \left\{ \frac{\partial}{\partial x} D_{0^+}^{1-\alpha} \theta_\alpha(x, t); s \right\} = -\frac{1}{2}, \quad \lim_{x \rightarrow 0^-} \mathcal{L} \left\{ \frac{\partial}{\partial x} D_{0^+}^{1-\alpha} \theta_\alpha(x, t); s \right\} = \frac{1}{2}, \quad (2.23)$$

$$\lim_{t \rightarrow 0} \theta_\alpha(x, t) = 0, \quad (2.24)$$

$$\lim_{x \rightarrow 1} \frac{\partial \theta_\alpha}{\partial x}(x, t) = 0. \quad (2.25)$$

where $H(t)$ and $G(t)$ are C^∞ on $[0, \infty)$ with all finite order derivatives vanishing at $t = 0$, i.e., $H^{(m)}(0) = G^{(m)}(0) = 0$. $(4\pi)^{-1/2} < c_0(\alpha) = \frac{1}{2\Gamma(1-\alpha/2)} < 1/2$ is a constant that only depends on α . \mathcal{L} denotes the Laplace transform and $D_{0^+}^{1-\alpha}$ is the Riemann-Liouville fractional derivative defined as in (2.1).

Note that like the normal diffusion case ($\alpha = 1$), the functions $H(t)$ and $G(t)$ are still infinitely differentiable and vanish, together with all orders of derivatives, at $t = 0$. The consequence of this is that the basic properties of our inverse problem with $\alpha < 1$ will remain the same although there will be quantitative differences for $\alpha < 1$ and $\alpha = 1$.

The first two equalities are direct and we will skip their proof and move to the proof of the relation (2.22).

Proof By direct calculation, for $m = 1, 2, \dots$ we obtain

$$\begin{aligned}\frac{\partial}{\partial x}(K_\alpha(x + 2m, t)) &= -\frac{1}{2}t^{-\alpha} \sum_{k=0}^{\infty} \frac{\left(-\frac{|x+2m|}{t^{\alpha/2}}\right)^k}{k!\Gamma(-\frac{\alpha}{2}k + (1 - \alpha))}, \\ \frac{\partial}{\partial x}(K_\alpha(x - 2m, t)) &= \frac{1}{2}t^{-\alpha} \sum_{k=0}^{\infty} \frac{\left(-\frac{|x-2m|}{t^{\alpha/2}}\right)^k}{k!\Gamma(-\frac{\alpha}{2}k + (1 - \alpha))}.\end{aligned}$$

Thus

$$\lim_{x \rightarrow 0^+} \left(\frac{\partial}{\partial x}(K_\alpha(x + 2m, t)) + \frac{\partial}{\partial x}(K_\alpha(x - 2m, t)) \right) = 0. \quad (2.26)$$

We now use the uniform convergence of series for θ_α and the equality (2.26) to obtain

$$\begin{aligned}\lim_{x \rightarrow 0^+} \frac{\partial \theta_\alpha(x, t)}{\partial x} &= \lim_{x \rightarrow 0^+} \frac{\partial}{\partial x} \left(\sum_{m=-\infty}^{\infty} K_\alpha(x + 2m, t) \right) = \lim_{x \rightarrow 0^+} \sum_{m=-\infty}^{\infty} \frac{\partial}{\partial x} (K_\alpha(x + 2m, t)) \\ &= \lim_{x \rightarrow 0^+} \sum_{m=1}^{\infty} \frac{\partial}{\partial x} (K_\alpha(x + 2m, t) + \frac{\partial}{\partial x} (K_\alpha(x - 2m, t))) + \lim_{x \rightarrow 0^+} \frac{\partial}{\partial x} (K_\alpha(x, t)) \\ &= \lim_{x \rightarrow 0^+} \frac{\partial}{\partial x} (K_\alpha(x, t)).\end{aligned}$$

This along with the series representation of K_α leads to the relation

$$\begin{aligned}\lim_{x \rightarrow 0^+} \frac{\partial \theta_\alpha(x, t)}{\partial x} &= \lim_{x \rightarrow 0^+} -\frac{1}{2}t^{-\alpha} \sum_{k=0}^{\infty} \frac{\left(-\frac{x}{t^{\alpha/2}}\right)^k}{k!\Gamma(-\frac{\alpha}{2}k + (1 - \alpha))} \\ &= \lim_{x \rightarrow 0^+} -\frac{1}{2}t^{-\alpha} W_{-\frac{\alpha}{2}, 1-\alpha}(x, t).\end{aligned}$$

Using the Laplace transform formula (see [22]) $\mathcal{L}\{t^{-\alpha} W_{-\frac{\alpha}{2}, 1-\alpha}; s\} = s^{-(1-\alpha)} \exp(-|x|s^{\alpha/2})$,

$$\lim_{x \rightarrow 0^+} \mathcal{L}\left\{ \frac{\partial \theta_\alpha(x, t)}{\partial x}; s \right\} = \lim_{x \rightarrow 0^+} -\frac{1}{2} s^{-(1-\alpha)} \exp(-|x|s^{\alpha/2}) = -\frac{1}{2} s^{\alpha-1},$$

which proves (2.22).

To prove (2.23), we show that the formula

$$\lim_{x \rightarrow 0^+} \int_0^t \frac{\partial}{\partial x} D_{0^+}^{1-\alpha} \theta_\alpha(x, t-\tau) \varphi(\tau) d\tau = -\frac{1}{2} \varphi(t) \quad (2.27)$$

holds for all $\varphi(t) \in C_0^\infty(0, \infty)$, and by Lemma 2.1.1, $D_{0^+}^{1-\alpha} \theta_\alpha(x, t)$ exists and is continuous for $x \in \mathbb{R}$ and $t > 0$, so that the Laplace transform formula $\mathcal{L}\{D_{0^+}^\alpha \varphi(t); s\} = s^\alpha \mathcal{L}\{\varphi(t); s\}$ is valid because $(D_{0^+}^{\alpha-1} \varphi(t))|_{t=0} = 0$. Taking the Laplace transform to the left hand side of (2.27) and using Lemma 2.4.2 we get the following chain of equalities

$$\begin{aligned} \lim_{x \rightarrow 0^+} \mathcal{L}\left\{\int_0^t \frac{\partial}{\partial x} D_{0^+}^{1-\alpha} \theta_\alpha(x, t-\tau) \varphi(\tau) d\tau; s\right\} &= \lim_{x \rightarrow 0^+} \mathcal{L}\left\{\int_0^t \frac{\partial}{\partial x} \theta_\alpha(x, t-\tau) D_{0^+}^{1-\alpha} \varphi(\tau) d\tau; s\right\} \\ &= \lim_{x \rightarrow 0^+} \mathcal{L}\left\{\frac{\partial}{\partial x} \theta_\alpha(x, t); s\right\} \times \mathcal{L}\left\{D_{0^+}^{1-\alpha} \varphi(t); s\right\} \\ &= -\frac{1}{2} s^{\alpha-1} \times s^{1-\alpha} \mathcal{L}\{\varphi(t); s\} \\ &= \mathcal{L}\left\{-\frac{1}{2} \varphi(t); s\right\}, \end{aligned}$$

which immediately gives (2.27).

To prove (2.24) we take $n = 1$, $m = 0$ in Proposition 1 in [18] (note that there is a terminology difference here; this reference uses the notation Z_0 in place of our θ_α). This gives the estimate $|\theta_\alpha| \leq Ct^{-\alpha/2} \exp(-\sigma t^{-\frac{\alpha}{2-\alpha}} |x|^{\frac{2}{2-\alpha}})$, so letting $t \rightarrow 0$ we obtain (2.24).

To show (2.25), we first calculate $\frac{\partial \theta_\alpha}{\partial x}(x, t)$ at the point $x = 1$ for $t > 0$:

$$\begin{aligned} \frac{\partial \theta_\alpha}{\partial x}(x, t) \Big|_{x=1} &= -\frac{1}{2} t^{-\alpha} \sum_{m=1}^{\infty} \sum_{k=0}^{\infty} \frac{\left(-\frac{[1+2m]}{t^{\alpha/2}}\right)^k}{k! \Gamma\left(-\frac{\alpha}{2}k + (1-\alpha)\right)} + \frac{1}{2} t^{-\alpha} \sum_{m=1}^{\infty} \sum_{k=0}^{\infty} \frac{\left(-\frac{[1-2m]}{t^{\alpha/2}}\right)^k}{k! \Gamma\left(-\frac{\alpha}{2}k + (1-\alpha)\right)} \\ &\quad - \frac{1}{2} t^{-\alpha} \sum_{k=0}^{\infty} \frac{\left(-\frac{1}{t^{\alpha/2}}\right)^k}{k! \Gamma\left(-\frac{\alpha}{2}k + (1-\alpha)\right)} = 0. \end{aligned}$$

Thus by the continuity of $\frac{\partial\theta_\alpha}{\partial x}(x, t)$ with respect to x , we get

$$\lim_{x \rightarrow 1} \frac{\partial\theta_\alpha}{\partial x}(x, t) = \frac{\partial\theta_\alpha}{\partial x}(x, t) \Big|_{x=1} = 0,$$

which gives (2.25). ■

The next lemma is needed in the proof of using the fixed point method to reconstruct the nonlinear source term in Section 4.

Lemma 2.4.4 *The relation $\lim_{t \rightarrow 0^+} \frac{\partial^2 D_{0^+}^{1-\alpha} \theta_\alpha}{\partial x^2}(x, t) = 0$ holds true for $0 < \alpha < 1$.*

Proof Let us denote the expression $D_{0^+}^{1-\alpha} \theta_\alpha(x, t)$ by $Y_0(t, x)$. This notation is used in equation (2.4) in [18], and then by Proposition 2 from [18] with $m = 2$ and $n = 1$ we obtain the estimate

$$\left| \frac{\partial^2 Y_0(x, t)}{\partial x^2} \right| \leq C t^{-1-\alpha/2} \exp(-\sigma t^{-\frac{\alpha}{2-\alpha}} |x|^{\frac{2}{2-\alpha}}).$$

where σ is a positive constant. We again note that [18] uses Z_0 in place of our θ_α .

Thus we get the estimate

$$\left| \frac{\partial^2 D_{0^+}^{1-\alpha} \theta_\alpha}{\partial x^2}(x, t) \right| \leq C t^{-1-\alpha/2} \exp(-\sigma t^{-\frac{\alpha}{2-\alpha}} |x|^{\frac{2}{2-\alpha}}),$$

from which the statement of lemma follows as $t \rightarrow 0$. ■

2.4.3 Unique existence and regularity

Let Ω be a bounded domain in \mathbb{R}^N with a sufficiently smooth boundary $\partial\Omega$. Let $L^2(\Omega)$ be a usual Lebesgue integrable space defined as in (1.2). $H^l(\Omega)$ and $H_0^m(\Omega)$

denote Sobolev spaces as defined in (1.8). In what follows, let L be given by

$$Lu(x) = \sum_{i=1}^N \frac{\partial}{\partial x_i} \left(\sum_{j=1}^N A_{ij}(x) \frac{\partial}{\partial x_j} u(x) \right) + C(x)u(x), \quad x \in \Omega,$$

where $A_{ij} = A_{ji}$, $1 \leq i, j \leq n$.

We assume that the operator L is uniformly elliptic on $\bar{\Omega}$ and that its coefficients are smooth: there exists a constant $\mu > 0$ such that

$$\sum_{j,j=1}^N A_{ij}(x) \xi_i \xi_j \geq \mu \sum_{i=1}^N \xi_i^2, \quad x \in \bar{\Omega}, \xi \in \mathbb{R}^n,$$

and the coefficients satisfy $A_{ij} \in C^1(\bar{\Omega})$, $C(x) \in C(\bar{\Omega})$, $C(x \leq 0, x \in \bar{\Omega})$.

We define an operator \bar{L} in $L^2(\Omega)$ by

$$(\bar{L}u)(x) = (Lu)(x), \quad x \in \Omega, \quad D(-\bar{L}) = H^2(\Omega) \cap H_0^1(\Omega).$$

Then the fractional power $(-\bar{L})^\gamma$ is defined for $\gamma \in \mathbb{R}$ and $D((-\bar{L})^{1/2}) = H_0^1(\Omega)$ for example. Henceforth we set $\|u\|_{D((-\bar{L})^\gamma)} = \|(-\bar{L})^\gamma u\|_{L^2(\Omega)}$. We note that the norm $\|u\|_{D((-\bar{L})^\gamma)}$ is stronger than $\|u\|_{L^2(\Omega)}$ for $\gamma > 0$.

Since $-\bar{L}$ is a symmetric uniformly elliptic operator, the spectrum of $-\bar{L}$ is entirely composed of eigenvalues. Counting according to the multiplicities, we can set: $0 < \lambda_1 \leq \lambda_2 \leq \dots$. By $\psi_n \in H^2(\Omega) \cap H_0^1(\Omega)$ we denote the orthonormal eigenfunction corresponding to $-\lambda_n$: $\bar{L}\psi_n = -\lambda_n\psi_n$.

We consider a time fractional diffusion equation,

$$\partial_t^\alpha u(x, t) - \bar{L}u(x, t) = \gamma(x, t), \quad x \in \Omega, t \in (0, T), 0 < \alpha < 1, \quad (2.28)$$

where $\gamma(x, t)$ is a given function on $\Omega \times (0, T)$ and ∂_t^α denotes the Caputo fractional

derivative ∂_{0+}^α defined as (2.4).

We will solve Equation (2.28) with the following initial/boundary value conditions:

$$u(x, t) = 0, \quad x \in \partial\Omega, t \in (0, T), \quad (2.29)$$

$$u(x, 0) = f(x), \quad x \in \Omega, \quad (2.30)$$

In ([53]), the authors give the following unique existence and regularity results for problem (2.28)-(2.30). For the sake of completeness, we list some here.

Definition 2.4.1 *We call u a weak solution to (2.28)-(2.30) if (2.28) holds in $L^2(\Omega)$ and $u(\cdot, t) \in H_0^1(\Omega)$ for almost all $t \in (0, T)$ and $u \in C([0, T]; D((-\bar{L})^{-\gamma}))$,*

$$\lim_{t \rightarrow 0} \|u(\cdot, t) - f(x)\|_{D((-\bar{L})^{-\gamma})} = 0$$

with some $\gamma > 0$.

Theorem 2.4.1 *Let $\gamma(x, t) = 0$, then*

- *Let $f \in L^2(\Omega)$. Then there exists a unique weak solution $u \in C([0, T]; L^2(\Omega)) \cap C((0, T]; H^2(\Omega) \cap H_0^1(\Omega))$ to (2.28)-(2.30) such that $\partial_t^\alpha u \in C((0, T]; L^2(\Omega))$. Moreover there exists a constant C_1 such that*

$$\begin{cases} \|u\|_{C([0, T]; L^2(\Omega))} \leq C_1 \|f\|_{L^2(\Omega)}, \\ \|u(\cdot, t)\|_{H^2(\Omega)} + \|\partial_t^\alpha u(\cdot, t)\|_{L^2(\Omega)} \leq C_1 t^{-\alpha} \|f\|_{L^2(\Omega)}. \end{cases}$$

and we have

$$u(x, t) = \sum_{n=1}^{\infty} (f, \psi_n) E_{\alpha, 1}(-\lambda_n t^\alpha) \psi_n(x) \quad (2.31)$$

in $C([0, T]; L^2(\Omega)) \cap C((0, T]; H^2(\Omega) \cap H_0^1(\Omega))$. Moreover $u : (0, T] \rightarrow L^2(\Omega)$ is analytically extended to a sector $\{z \in \mathbb{C}; z \neq 0, |\arg z| < \frac{1}{2}\pi\}$.

- We assume that $f \in H^2(\Omega)$. Then the unique weak solution u further belongs to $L^2((0, T]; H^2(\Omega \cap H_0^1(\Omega)))$, $\partial_t \alpha u \in L^2(\Omega \times (0, T))$ and there exists a constant $C_2 > 0$ satisfying the following inequality:

$$\|u\|_{L^2((0, T]; H^2(\Omega))} + \|\partial_t^\alpha u\|_{L^2(\Omega \times (0, T))} \leq C_2 \|f\|_{H^1(\Omega)} \quad (2.32)$$

and we have (2.31) in the corresponding space on the right hand side of (2.32).

- We assume that $f \in H^2(\Omega) \cap H_0^1(\Omega)$. Then the unique solution u belongs to $C((0, T]; H^2(\Omega \cap H_0^1(\Omega)))$, $L^2((0, T]; H^2(\Omega \cap H_0^1(\Omega)))$, $\partial_t \alpha u \in C([0, T]; L^2(\Omega) \cap C(\times(0, T); H_0^1(\Omega)))$ and the following inequality holds:

$$\|u\|_{C((0, T]; H^2(\Omega))} + \|\partial_t^\alpha u\|_{C((0, T]; L^2(\Omega))} \leq C_3 \|f\|_{H^2(\Omega)} \quad (2.33)$$

and we have (2.31) in the corresponding space on the right hand side of (2.33).

Theorem 2.4.2 *Let $f = 0$ and $\gamma \in L^\infty((0, T]; L^2(\Omega))$. Then there exists a unique weak solution $u \in L^2((0, T]; H^2(\Omega) \cap H_0^1(\Omega))$ to (2.28)-(2.30) such that $\partial_t^\alpha u \in L^2((0, T] \times \Omega)$. In particular, for any $\gamma > \frac{N}{4} - 1$, we have $u \in C([0, T]; D((-\bar{L})^{-\gamma}))$,*

$$\lim_{t \rightarrow 0} \|u(\cdot, t)\|_{D((-\bar{L})^{-\gamma})} = 0,$$

and if $n = 1, 2, 3$, then

$$\lim_{t \rightarrow 0} \|u(\cdot, t)\|_{L^2(\Omega)} = 0.$$

Moreover, there exists a constant $C_4 > 0$ such that

$$\|u\|_{L^2(0, T; H^2(\Omega))} + \|\partial_t^\alpha u\|_{L^2(\Omega \times (0, T))} \leq C_4 \|\gamma\|_{L^2(\Omega \times (0, T))}. \quad (2.34)$$

and we have

$$u(x, t) = \sum_{n=1}^{\infty} \left(\int_0^t (\gamma(\cdot, \tau), \psi_n) (t - \tau)^{\alpha-1} E_{\alpha, \alpha}(-\lambda_n (t - \tau)^\alpha) d\tau \right) \psi_n(x) \quad (2.35)$$

in the corresponding space on the right hand side of (2.34).

Theorem 2.4.3 *Let $f \in H^2(\Omega) \cap H_0^1(\Omega)$ and $\gamma(x, t) \in C^\theta([0, T]; L^2(\Omega))$. Then for the solution u given by*

$$u(x, t) = \sum_{n=1}^{\infty} \left\{ (f, \psi_n) E_{\alpha, 1}(-\lambda_n t^\alpha) + \int_0^t (\gamma(\cdot, \tau), \psi_n) (t - \tau)^{\alpha-1} E_{\alpha, \alpha}(-\lambda_n (t - \tau)^\alpha) d\tau \right\} \psi_n(x), \quad (2.36)$$

we have

- For every $\delta > 0$,

$$\|\bar{L}u\|_{C^\theta([\delta, T]; L^2(\Omega))} + \|\partial_t^\alpha u\|_{C^\theta([\delta, T]; L^2(\Omega))} \leq \frac{C_5}{\delta} (\|\gamma\|_{C^\theta([\delta, T]; L^2(\Omega))} + \|f\|_{H^2(\Omega)}).$$

-

$$\|\bar{L}u\|_{C([0, T]; L^2(\Omega))} + \|\partial_t^\alpha u\|_{C([0, T]; L^2(\Omega))} \leq \frac{C_6}{\delta} (\|\gamma\|_{C^\theta([0, T]; L^2(\Omega))} + \|f\|_{H^2(\Omega)}).$$

- If $f = 0$ and $\gamma(\cdot, 0) = 0$, then

$$\|\bar{L}u\|_{C^\theta([0, T]; L^2(\Omega))} + \|\partial_t^\alpha u\|_{C^\theta([0, T]; L^2(\Omega))} \leq \frac{C_7}{\delta} (\|\gamma\|_{C^\theta([0, T]; L^2(\Omega))} + \|f\|_{H^2(\Omega)}).$$

Theorem 2.4.4 *Let $f \in L^2(\Omega)$ and $\gamma = 0$. Then for the unique weak solution $u \in C([0, \infty]; L^2(\Omega)) \cap C((0, \infty]; H^2(\Omega) \cap H_0^1(\Omega))$ to (2.28)-(2.30), there exists a*

constant $C_8 > 0$ such that

$$\|u(\cdot, t)\|_{L^2(\Omega)} \leq \frac{C_8}{1 + \lambda_1 t^\alpha} \|f\|_{L^2(\Omega)}, \quad t \geq 0.$$

Moreover there exists a constant C_9 such that

$$u \in C^\infty((0, \infty); L^2(\Omega)), \quad \|\partial_t^m u(\cdot, t)\|_{L^2(\Omega)} \leq \frac{C_9}{t^m} \|f\|_{L^2(\Omega)}, \quad t > 0, m \in \mathbb{N}. \quad (2.37)$$

Remark 2.4.1 • For fractional diffusion equations, we do not have smoothing properties like the classical diffusion equation as we discussed in Theorem 1.4.2. For $\gamma = 0$, there is the smoothing property in space with order 2, which means that $u(\cdot, t) \in H^2(\Omega)$ for any $t > 0$ and any $u(\cdot, 0) \in L^2(\Omega)$, while (2.37) means that the regularity in time immediately becomes stronger in t , and is of the infinity order (u is of C^∞ for $t > 0$).

- When $f = 0$, estimate (2.34) is the corresponding regularity of the solution to the classical case.
- Theorem 2.4.3 means that the same regularity results hold for the nonhomogeneous equation in the classical case.

For more existence and uniqueness results of Problem (2.28)-(2.30) under different assumptions of f, g and γ , we can refer to [53].

2.4.4 Weak maximum principle

In [36], the author proved the following (weak) maximum principle for the generalized time-fractional diffusion equation (Theorem 2 in [36]). Since it is critical for our further discussion, we list it here.

Theorem 2.4.5 *Let a function $u \in C(\Omega \times [0, T]) \cap H^{1,2}(0, T) \cap C^2(\Omega)$ be a solution of the fractional diffusion equation (2.28) with $c(x) \geq 0$, $\gamma(x, t) \leq 0$, $(x, t) \in \Omega \times [0, T]$. Then either $u(x, t) \leq 0$ or the function u attains its positive maximum on the bottom or back-side parts $S(S := (\Omega \times \{0\}) \cup (\partial\Omega \times [0, T]))$ of the boundary of the domain $\Omega \times [0, T]$, i.e.,*

$$u(x, t) \leq \max\{0, \max_{(x,t) \in S} u(x, t)\}, \quad \forall x \in \Omega \times [0, T].$$

Note this is the *weak* maximum principle. The counterpart of the strong maximum principle as discussed in Theorem 1.4.3 is still open.

2.4.5 Solution for Dirichlet boundary conditions

The θ_α -function is now used to obtain a representation for a solution of the direct problem with Dirichlet boundary conditions and initial conditions.

Lemma 2.4.5 *Let u_0 , g_1 , and g_2 be piecewise-continuous functions. Then a solution u of the initial-boundary-value problem for the fractional reaction-diffusion problem given by*

$$\begin{cases} \partial_t^\alpha u - u_{xx} = f(u) + \gamma(x, t), & 0 < x < 1, 0 < t < T \\ u(x, 0) = u_0(x), & 0 < x < 1, \\ u(0, t) = g_1(t), \quad u(1, t) = g_2(t), & 0 \leq t \leq T \end{cases} \quad (2.38)$$

can be represented in the form

$$u(x, t) = w(x, t) + v_1(x, t) + v_2(x, t) + v_3(x, t), \quad (2.39)$$

where

$$\begin{aligned}
w(x, t) &= \int_0^1 \left[\theta_\alpha(x - \xi, t) + \theta_\alpha(x + \xi, t) \right] u_0(\xi) d\xi, \\
v_1 &= -2 \int_0^t \frac{\partial(D_{0+}^{1-\alpha} \theta_\alpha)}{\partial x}(x, t - \tau) g_1(\tau) d\tau, \\
v_2 &= -2 \int_0^t \frac{\partial(D_{0+}^{1-\alpha} \theta_\alpha)}{\partial x}(x - 1, t - \tau) g_2(\tau) d\tau, \\
v_3 &= \int_0^t \int_0^1 \left[(D_{0+}^{1-\alpha} \theta_\alpha)(x - \xi, t - \tau) + (D_{0+}^{1-\alpha} \theta_\alpha) \theta_\alpha(x + \xi, t - \tau) \right] [f(u(\xi, \tau) + \gamma(\xi, \tau))] d\xi d\tau.
\end{aligned}$$

Proof By the definition of θ_α -function, we have

$$\begin{aligned}
\partial_t^\alpha w &= \int_0^1 \left[\partial_t^\alpha \theta_\alpha(x + \xi, t) + \partial_t^\alpha \theta_\alpha(x - \xi, t) \right] u_0(\xi) d\xi \\
&= \int_0^1 \left[\theta_\alpha(x + \xi, t) + \theta_\alpha(x - \xi, t) \right]_{xx} u_0(\xi) d\xi = w_{xx}.
\end{aligned}$$

Then by direct calculation we get the following chain of equalities:

$$\begin{aligned}
\partial_t^\alpha v_1 &= -2 \partial_t^\alpha \left(\int_0^t D_{0+}^{1-\alpha} \left(\frac{\partial \theta_\alpha}{\partial x} \right) (x, t - \tau) g_1(\tau) d\tau \right) \\
&= -2 \partial_t^\alpha \left(\int_0^t \frac{\partial \theta_\alpha}{\partial x} (x, t - \tau) D_{0+}^{1-\alpha} g_1(\tau) d\tau \right) \\
&= -2 \left(\int_0^t \frac{\partial}{\partial x} (\partial_t^\alpha \theta_\alpha)(x, t - \tau) D_{0+}^{1-\alpha} g_1(\tau) d\tau \right) \\
&= -2 \left(\int_0^t \frac{\partial}{\partial x} ((\theta_\alpha)_{xx})(x, t - \tau) D_{0+}^{1-\alpha} g_1(\tau) d\tau \right) \\
&= -2 \left(\int_0^t D_{0+}^{1-\alpha} \left(\frac{\partial \theta_\alpha}{\partial x} \right)_{xx} (x, t - \tau) g_1(\tau) d\tau \right) \\
&= -2 \left(\int_0^t \left(\frac{\partial D_{0+}^{1-\alpha} \theta_\alpha}{\partial x} \right)_{xx} (x, t - \tau) g_1(\tau) d\tau \right) \\
&= \left(-2 \int_0^t \frac{\partial(D_{0+}^{1-\alpha} \theta_\alpha)}{\partial x} (x, t - \tau) g_1(\tau) d\tau \right)_{xx} = (v_1)_{xx},
\end{aligned}$$

where we change the order of $D_{0+}^{1-\alpha}$ and $\frac{\partial}{\partial x}$ several times, which is guaranteed because

of the uniform convergence of θ_α and its fractional derivatives.

Using the same technique, we obtain the equation $\partial_t^\alpha v_2 = (v_2)_{xx}$, then following the Duhamel principle for the fractional order equations that was formulated in [56], we can get v_3 is a solution to the following problem

$$\begin{cases} \partial_t^\alpha v - v_{xx} = f(v) + \gamma(x, t), & 0 < x < 1, 0 < t < T, \\ v(x, 0) = 0, & 0 < x < 1, \\ v(0, t) = 0, \quad -v(1, t) = 0, & 0 \leq t \leq T. \end{cases} \quad (2.40)$$

To verify the initial condition, we just substitute $t = 0$ in the formula (2.39).

The fact that (2.39) satisfies the boundary conditions can be proved from the formulas (2.23)-(2.25) in Lemma 2.4.3, we just take v_1 for example.

On the left boundary, $x = 0$, we have

$$\lim_{x \rightarrow 0^+} v_1(x, t) = -2 \lim_{x \rightarrow 0^+} \int_0^t \frac{\partial}{\partial x} (D_{0^+}^{1-\alpha} \theta_\alpha)(x, t-\tau) g_1(\tau) d\tau = g_1(x, t),$$

where in the last equality we applied (2.23) in Lemma 2.4.3.

On the right boundary, $x = 1$, we have

$$\lim_{x \rightarrow 1^-} v_1(x, t) = -2 \int_0^t D_{0^+}^{1-\alpha} \left(\lim_{x \rightarrow 1^+} \frac{\partial}{\partial x} (\theta_\alpha(x, t-\tau)) \right) g_1(\tau) d\tau = 0,$$

where we applied equation (2.25) from Lemma 2.4.3. ■

2.4.6 Solution for Neumann boundary conditions

Lemma 2.4.6 *Let u_0 , g_1 , and g_2 be piecewise-continuous functions. Then a solution u of the initial-boundary-value problem*

$$\begin{cases} \partial_t^\alpha u - u_{xx} = f(u) + \gamma(x, t), & 0 < x < 1, 0 < t < T \\ u(x, 0) = u_0(x), & 0 < x < 1, \\ u_x(0, t) = g_1(t), \quad -u_x(1, t) = g_2(t), & 0 \leq t \leq T \end{cases} \quad (2.41)$$

can be represented in the form

$$u(x, t) = w(x, t) + v_1(x, t) + v_2(x, t) + v_3(x, t), \quad (2.42)$$

where

$$\begin{aligned} w(x, t) &= \int_0^1 [\theta_\alpha(x-\xi, t) + \theta_\alpha(x+\xi, t)] u_0(\xi) d\xi, \\ v_1 &= -2 \int_0^t (D_{0+}^{1-\alpha} \theta_\alpha)(x, t-\tau) g_1(\tau) d\tau, \\ v_2 &= 2 \int_0^t (D_{0+}^{1-\alpha} \theta_\alpha)(x-1, t-\tau) g_2(\tau) d\tau, \\ v_3 &= \int_0^t \int_0^1 [(D_{0+}^{1-\alpha} \theta_\alpha)(x-\xi, t-\tau) + (D_{0+}^{1-\alpha} \theta_\alpha)(x+\xi, t-\tau)] [f(u(\xi, \tau) + \gamma(\xi, \tau)] d\xi d\tau. \end{aligned}$$

Proof We first verify the governing equation $\partial_t^\alpha u(x, t) = \partial_t^\alpha w + \partial_t^\alpha v_1 + \partial_t^\alpha v_2 + \partial_t^\alpha v_3$, noting that both the identity $\partial_t^\alpha w = w_{xx}$ and the equation satisfied by v_3 have previously been verified in Lemma 2.4.5. Then by direct calculation we get the following chain of equalities where we use the fact that $\theta_\alpha(x, 0) = 0$ (which follows

from Lemma 2.4.3):

$$\begin{aligned}
\partial_t^\alpha v_1 &= -2\partial_t^\alpha \left(\int_0^t (D_{0+}^{1-\alpha} \theta_\alpha)(x, t-\tau) g_1(\tau) d\tau \right) \\
&= -2\partial_t^\alpha \left(\int_0^t \theta_\alpha(x, t-\tau) D_{0+}^{1-\alpha} g_1(\tau) d\tau \right) \\
&= -\frac{2}{\Gamma(1-\alpha)} \int_0^t \frac{1}{(t-s)^\alpha} \left(\theta_\alpha(x, 0) D_{0+}^{1-\alpha} g_1(s) + \int_0^s \frac{\partial \theta_\alpha}{\partial s}(x, s-\tau) D_{0+}^{1-\alpha} g_1(\tau) d\tau \right) ds \\
&= -\frac{2}{\Gamma(1-\alpha)} \int_0^t \int_0^s \frac{1}{(t-s)^\alpha} \frac{\partial \theta_\alpha}{\partial s}(x, s-\tau) D_{0+}^{1-\alpha} g_1(\tau) d\tau ds \\
&= -\frac{2}{\Gamma(1-\alpha)} \int_0^t \int_\tau^t \frac{1}{(t-s)^\alpha} \frac{\partial \theta_\alpha}{\partial s}(x, s-\tau) ds D_{0+}^{1-\alpha} g_1(\tau) d\tau \\
&= -\frac{2}{\Gamma(1-\alpha)} \int_0^t \int_0^{t-\tau} \frac{1}{(t-\tau-\mu)^\alpha} \frac{\partial \theta_\alpha}{\partial \mu}(x, \mu) d\mu D_{0+}^{1-\alpha} g_1(\tau) d\tau \\
&= -2 \int_0^t \partial_t^\alpha \theta_\alpha(x, t-\tau) D_{0+}^{1-\alpha} g_1(\tau) d\tau = -2 \int_0^t [\theta_\alpha(x, t-\tau)]_{xx} D_{0+}^{1-\alpha} g_1(\tau) d\tau \\
&= \left(-2 \int_0^t D_{0+}^{1-\alpha} \theta_\alpha(x, t-\tau) g_1(\tau) d\tau \right)_{xx} = (v_1)_{xx}.
\end{aligned}$$

Using the same technique, we obtain the equality $\partial_t^\alpha v_2 = (v_2)_{xx}$ and thus we arrive at the formula (2.42).

To verify the initial condition from (2.41), we just substitute $t = 0$ in the formula (2.42).

The fact that (2.42) satisfies the boundary conditions from (2.41) can be proved using the formulas (2.23)-(2.25) from Lemma 2.4.3. For example, let us consider the part v_1 of the solution u .

On the left hand boundary $x = 0$,

$$\lim_{x \rightarrow 0+} \frac{\partial}{\partial x} (v_1(x, t)) = -2 \lim_{x \rightarrow 0+} \int_0^t \frac{\partial}{\partial x} (D_{0+}^{1-\alpha} \theta_\alpha)(x, t-\tau) g_1(\tau) d\tau = g_1(x, t).$$

In the last equality, the formula (2.23) from Lemma 2.4.3 was applied.

On the right hand boundary, $x = 1$,

$$\lim_{x \rightarrow 1^-} \frac{\partial}{\partial x} (v_1(x, t)) = -2 \int_0^t D_{0+}^{1-\alpha} \lim_{x \rightarrow 1+} \frac{\partial}{\partial x} (\theta_\alpha(x, t-\tau)) g_1(\tau) d\tau = 0$$

follows from formula (2.25) in Lemma 2.4.3. ■

2.5 Numerical evaluations

2.5.1 Evaluation of Wright function

We have the following integral representation for the Wright function (1.29) ([57]-[60]),

$$W_{\alpha, \beta}(z) = \frac{1}{2\pi i} \int_{\gamma(\varepsilon)} e^{(\zeta+z\zeta^{-\alpha})} \zeta^{-\beta} d\zeta, \quad \alpha > -1, \beta \in \mathbb{R}, \quad (2.43)$$

where $\gamma(\varepsilon)$ denotes the Hankel path in the z -plane with a cut along the negative real semi-axis $\arg(\zeta) = \pi$. In what follows we restrict ourselves to the numerical evaluation of the Wright function with the real negative arguments because this case is the most important for our further discussions.

In [34], the author has the following result.

Theorem 2.5.1 *Let $z = -x$, $x > 0$. Then the Wright function $W_{\alpha, \beta}(z)$ has the following integral representation depending on its parameter α and β :*

$$W_{\alpha, \beta}(z) = \frac{1}{\pi} \int_0^{+\infty} K(\alpha, \beta, x, r) dr, \quad (2.44)$$

if $(-1 < \alpha < 0$ and $\beta < 1)$ or $0 < \alpha < 1/2$ or $(\alpha = 1/2$ and $\beta < 1 + \alpha)$,

$$W_{\alpha, \beta}(z) = e + \frac{1}{\pi} \int_0^{+\infty} K(\alpha, \beta, x, r) dr, \quad (2.45)$$

if $(-1 < \alpha < 0$ and $\beta = 1)$,

$$W_{\alpha,\beta}(z) = \frac{1}{\pi} \int_1^{+\infty} K(\alpha, \beta, x, r) dr + \frac{1}{\pi} \int_0^\pi \tilde{P}[\alpha, \beta, x, \varphi] d\varphi, \quad (2.46)$$

in all other cases, with

$$K(\alpha, \beta, x, r) = e^{-r-xr^{-\alpha} \cos(\pi\alpha)} r^{-\beta} \sin(-xr^{-\alpha} \sin(\pi\alpha) + \pi\beta),$$

$$\tilde{P}[\alpha, \beta, x, \varphi] = e^{\cos(\varphi)-x \cos(\alpha\varphi)} \cos(\sin(\varphi) + x \sin(\pi\varphi) + \varphi(1 - \beta)).$$

The proof can be found in [36].

2.5.2 Finite difference scheme for fractional diffusion equations

We use the following direct solver to obtain the the solution $u(x, t)$ to equation (2.28) with various initial/boundary conditions in the one-dimensional space case, without loss of generality, we assume the domain we are interested in is $x \in [0, 1]$, $t \in [0, 1]$. This is based on the fractional derivative implicit time step method derived from [33] with modifications to take into account the boundary conditions.

Let x_j and t_k be the uniformly spaced grid points on $x \in [0, 1]$, $t \in [0, 1]$ and Δx and Δt the space and time step size. Thus we write $u_j^{k+1} = u(x_j, t_{k+1})$. For the fractional time derivative, we use

$$\partial_t^\alpha u^{k+1}(x) \approx \frac{1}{\Gamma(2 - \alpha)} \sum_{j=0}^k b_j \frac{u(x, t_{k+1-j}) - u(x, t_{k-j})}{\Delta t^\alpha}, \quad (2.47)$$

where the weights $b_j = (j + 1)^{1-\alpha} - j^{1-\alpha}$, $j = 0, 1, \dots, k$ form a monotone sequence converging to 0. It was proven in [33] that this finite difference scheme for time fractional derivatives has a convergence rate of $\Delta t^{2-\alpha}$.

From (2.47) we can see that to calculate the fractional derivative of $u(x, t)$ at

$t = t_{k+1}$, we need to store all the values of $u(x, t_j)$ for $j = 0, 1, \dots, k + 1$, and we need to add them up one by one, which requires both additional storage and time as we discussed in Section 2.3.3.

For the space derivative, we use the usual central difference scheme.

$$\frac{\partial^2}{\partial x_j^2} u(x_j, t_{k+1}) = \frac{u_{j-1}^{k+1} - 2u_j^{k+1} + u_{j+1}^{k+1}}{\Delta x^2}, \quad (2.48)$$

Combining (2.47) and (2.48) we obtain

$$u^{k+1} - \alpha_0 \frac{u_{j-1}^{k+1} - 2u_j^{k+1} + u_{j+1}^{k+1}}{\Delta x^2} = (1 - b_1)u^k + \sum_{j=1}^{k-1} (b_j - b_{j+1})u^{k-j} + b_k u^0, \quad k \geq 1$$

where $\alpha_0 = \Gamma(2 - \alpha)\Delta t^\alpha$.

If the boundary condition is of the Neumann type with nonlinear dependence, we have $\frac{u_1^{k+1} - u_{-1}^{k+1}}{2\Delta x} = f(u_0^{k+1})$ and we solve this nonlinear equation by iteration. This is achieved by lagging the argument of f . Initially we take $u_{-1}^{k+1} - u_1^{k+1} = 2\Delta x f(u_0^k)$ and back-substitute to obtain an approximation \tilde{u}^{k+1} . We then repeat with $u_{-1}^{k+1} - u_1^{k+1} = 2\Delta x f(\tilde{u}_0^{k+1})$ and iterate until effective convergence of u^{k+1} is obtained. In practice this step must only be repeated for a few times although the amount will clearly depend on the function f . This is a standard technique for the numerical solution of parabolic problems (Chapter 17 in [51]) that we have adapted.

2.5.3 Smoothing spline interpolation

For given data $\{x_i, y_i\}, i = 1, 2, \dots, N$, we want to find the function f that satisfies

$$\min_{f \in \mathcal{U}} \|f(x_i) - y_i\|_{l^2}, \quad (2.49)$$

where U is the specific function space we choose. When we use polynomials of degree three as the local basis for U in expressing the function $f(x)$, it is called cubic spline interpolation.

Sometimes, the given data set $\{y_i\}$ contains errors so that the interpolation through the data points given by (2.49) leads to highly oscillatory solutions that we do not believe adequately represent f . The smoothing spline, which minimizes

$$\lambda \sum_{j=1}^N \|y_j - f(x_j)\|_{l^2} + (1 - \lambda) \|f''(x)\|_{L^2}, \quad (2.50)$$

where $\|\cdot\|_{l^2}$ is the norm defined by (1.1), N is the number of entries of x , and the L^2 norm defined as (1.2) is evaluated over the smallest interval containing all the entries of x . λ is the smoothing parameter and it determines the relative weight placed on the contradictory demands of having $f(x)$ be smooth versus having $f(x)$ interpolate the data. For $\lambda = 0$, $f(x)$ is the least-square straight line fit to the data, while, at the other extreme, i.e., for $\lambda = 1$, f is the variational, or ‘natural’ cubic spline interpolant. As λ moves from 0 to 1, the smoothing spline changes from one extreme to the other. For more information about Cubic splines, see Section 3.3 in [51].

3. INVERSE BOUNDARY PROBLEMS FOR FRACTIONAL DIFFUSION EQUATIONS*

As we saw in the last section, whereas direct problems for fractional diffusion equations are well covered in the literature, research on inverse problems is less abundant. One of the most interesting aspects regarding inverse problems for fractional differential equations is the non-local character of fractional derivatives that often leads to significant changes of outcome when compared to the equivalent problems for classical derivatives. From Section 2.3.1 and Section 2.3.2, we see there are radical differences. For example, the fact that the local behavior of the time derivative shows that in a series of time steps, the solution depends only on the previous step, so that the history of the initial data is quickly lost. In contrast, the fractional diffusion problem carries information about all previous time steps. There are also some cases known, where qualitative properties of the inverse problems in the fractional case mirror those for the equations with integer order derivatives. For example, uniqueness for a one-dimensional time-fractional diffusion equation of the fractional order and of the diffusion coefficient was proven in [10] and uniqueness of a potential resulting from the multiple input sources was proven in [29].

We investigate an inverse boundary problem that seeks to reconstruct the exact form of the unknown boundary conditions under the assumption that the heat flux across the boundary is a function only of temperature. The unknown Neumann boundary condition is $\frac{\partial u}{\partial \nu} = f(u)$ for some function f that has to be determined, where ν is the unit outward norm.

*Portions of this section are reprinted with permission from "The determination of an unknown boundary condition in a fractional diffusion equation" by William Rundell, Xiang Xu and Lihua Zuo, *Applicable Analysis* (2012) DOI:10.1080/00036811.2012.686605, Copyright [2012] by Taylor& Francis.

In the case of a purely conductive process over a narrow range of temperatures the usual condition taken is Newton's law of cooling: $f(u) = a(u - u_0)$ with u_0 being the ambient temperature. For a purely radiative process the Stefan-Boltzmann law $f(u) = b(u^4 - u_0^4)$ is the usual ansatz. In the case of cooling from high temperatures (for example in steelmaking), the radiative condition is the dominant process at high temperatures: the conductive condition dominates as the steel nears the ambient temperature. In this context, our inverse problem is thus one of determining the exact form of the cooling process as a function of temperature.

Of course, in the case of normal heat conduction this is not a new problem. Pilant and Rundell [45]- [49] gave uniqueness results and proposed an iterative method to determine an unknown boundary condition in the case of the heat equation. Here we also consider the one spatial dimensional situation and generalize the result in [45] to a fractional diffusion equation, i.e., to establish the existence and uniqueness of the solution to the following inverse problem:

$$\partial_t^\alpha u - u_{xx} = 0, \quad 0 < x < 1, \quad 0 < t < T, \quad (3.1)$$

$$u(x, 0) = u_0(x), \quad 0 < x < 1, \quad (3.2)$$

with either of the nonlinear Neumann boundary conditions

$$u_x(0, t) = f(u(0, t)), \quad -u_x(1, t) = f(u(1, t)), \quad 0 \leq t \leq T, \quad (3.3)$$

or

$$u_x(0, t) = g(t), \quad -u_x(1, t) = f(u(1, t)), \quad 0 \leq t \leq T, \quad (3.4)$$

together with measured data, which we take to be the value of the temperature at

the left hand endpoint

$$u(0, t) = h(t), \quad 0 \leq t \leq T. \quad (3.5)$$

Here $f(\cdot)$ is unknown but depends only on the temperature of the corresponding boundary, and ∂_t^α ($0 < \alpha < 1$) is the fractional derivative in the Caputo sense, which is defined as (2.4).

The exact value of α may also be unknown and the determination of this quantity could be viewed as part of the inverse problem - which then amounts to the determination of the pair $\{\alpha, f\}$ from the overposed data $h(t)$. However, the determination of α turns out to be quite nontrivial and becomes impossible, at least using the method we present here.

While we will follow the ideas of [45], there are several obstacles to be overcome before these techniques can be applied. Even for the direct problem for the heat equation ($\alpha = 1$), some a priori assumptions on f are required. For example, if $f > 0$ then we are sending in heat flux through one or both boundaries and the nonlinearity can cause the temperature $u(x, t)$ to blow-up in finite time. For the heat equation this cannot happen if $f < 0$ and we are in a cooling situation; the solution $u(x, t)$ is then bounded by $\sup |u_0(x)|$. We must establish similar properties for (3.1) – (3.4) in order to utilize information about the direct problem. In the case of (3.4) and $\alpha = 1$, uniqueness of the function f follows from unique continuation of the Cauchy data on $x = 0$ to obtain $u(x, t)$ for $x > 0$ and hence both $u(1, t)$ and $u_x(1, t)$, from which there can be at most one f within the range of $u(1, t)$. Of course, this so called “sideways heat problem” is notoriously ill-posed and this approach is very definitely *not* the way to attempt a reconstruction of f . Moreover, in the case of $\alpha < 1$, which we will see in the next section that the structure of the analytic kernel still allows this unique continuation property to hold, it is another issue whether the

resulting degree of ill-posedness remains the same. Regardless, we should seek an alternative approach.

Our method will be to utilize the fundamental solution for a fractional diffusion equation in free space, constructing a closed form analytical solution for (3.1). Then incorporating the additional boundary data into this solution gives an integral equation of the generalized Abel type with unknown function $f(u)$. By applying the well-known inversion formula for such equations, we obtain an integral equation of the second kind with a weakly singular kernel involving numerical differentiation of the overposed boundary data. The existence and uniqueness of recovering $f(u)$ can then be obtained by a fixed point argument. This will require some regularity conditions on the boundary data. For the numerical differentiation step, we require regularization and we do so by using a smoothing spline tailored to the conditions of the problem. Numerical experiments demonstrate that this method gives an efficient way to reconstruct the unknown boundary condition $f(u)$.

The remainder of this section is organized as follows. Section 3.1 is devoted to the problem formulation, the properties of the fundamental solution and the associated M function for (3.1). We also prove the existence and uniqueness of the solution by using a fixed point argument for a nonlinear Volterra integral equation. Based on the inversion formula obtained for this Volterra equation, we construct the regularized solution for the unknown boundary condition $f(u)$. Numerical examples are presented to illustrate the validity of this method in Section 3.2.

We make the following assumptions on the data functions $u_0(x)$, $h(t)$ and the unknown flux-temperature model function f .

- A0 The unknown $f(\cdot)$ is a Lipschitz continuous function with uniform sign: $f > 0$ for the case of a heating model and $f < 0$ for the cooling case.

A1 In the case of (3.4) the imposed flux g has the same regularity assumption with f and of fixed sign on $(0, T)$.

A2 $u_0(x) \in C[0, 1]$.

A3 The overposed data $h(t)$ is monotone and continuously differentiable on $[0, T]$ with $h'(t) \in C[0, T]$ and the compatibility condition $h(0) = u_0(0)$.

We consider the functions with a $(1 - \frac{\alpha}{2})$ th order derivative on the interval $[0, T]$, and use the symbol \mathcal{H} for this space, setting

$$|f|_{\mathcal{H}} = \sup_{0 \leq t_1 < t_2 \leq T} \frac{|f(t_1) - f(t_2)|}{|t_1 - t_2|^{1-\alpha/2}}$$

as the usual seminorm, and $\|\cdot\|_{\mathcal{H}} = |\cdot|_{\mathcal{H}} + \|\cdot\|_{\infty}$ as the norm.

Remark 3.0.1 *The monotonicity of $h(t)$ is essential and the sign restrictions of u_0 , f (or g in the case of (3.4)) impose this.*

3.1 Existence and uniqueness

Lemma 3.1.1 *There exists a solution to the forward problem (3.1)-(3.4).*

Proof In Lemma (2.4.5), set $f(u) = 0, \gamma(x, t) = 0$ and replace $g_1(t)$ and $g_2(t)$ with $f(u(0, t))$ (or $g(t)$ in (3.4) case) and $f(u(1, t))$ respectively. ■

Lemma 3.1.2 *The overposed data $h(t)$ satisfies:*

$$\begin{aligned} h(t) = & \int_0^1 \left[\theta_{\alpha}(\xi, t) + \theta_{\alpha}(-\xi, t) \right] u_0(\xi) d\xi \\ & - 2 \int_0^t (D_{0+}^{1-\alpha} \theta_{\alpha})(0, t - \tau) f(h(\tau)) d\tau - 2 \int_0^t (D_{0+}^{1-\alpha} \theta_{\alpha})(-1, t - \tau) f(u(1, \tau)) d\tau. \end{aligned} \tag{3.6}$$

Let

$$\begin{aligned} k(t) &= \frac{1}{2}(w(0, t) - u(0, t)) - \int_0^t D_{0+}^{1-\alpha} \theta_\alpha(-1, t - \tau) f(u(1, \tau)) d\tau \\ &= \frac{1}{2}(w(0, t) - u(0, t)) - \int_0^t D_{0+}^{1-\alpha} G(t - \tau) f(u(1, \tau)) d\tau. \end{aligned}$$

Then $f(h(\tau))$ is the solution of the integral equation $\int_0^t D_{0+}^{1-\alpha} \theta_\alpha(0, t - \tau) f(h(\tau)) = k(t)$ which can be written in the form

$$c_1(\alpha) \int_0^t \frac{f(h(\tau))}{(t - \tau)^{1-\alpha/2}} d\tau + \int_0^t H^{1-\alpha}(t - \tau) f(h(\tau)) d\tau = k(t), \quad (3.7)$$

where $c_1(\alpha) = \frac{c_0(\alpha)\Gamma(1-\alpha/2)}{\Gamma(\alpha/2)} = \frac{1}{2\Gamma(\alpha/2)}$ is a positive constant, and $H^{1-\alpha}(t) = D_{0+}^{1-\alpha} H(t) \in C^\infty([0, \infty))$.

Lemma 3.1.3 *If $k(t)$ is absolutely continuous, with $k'(t) \in L^\infty(0, T)$, then the solution of (3.7) satisfies*

$$f(h(t)) = c_2(\alpha) \left\{ \int_0^t \frac{k'(\tau)}{(t - \tau)^{\alpha/2}} d\tau - \int_0^t f(h(\eta)) \int_\eta^t \frac{(H^{1-\alpha})'(\tau - \eta)}{(t - \tau)^{\alpha/2}} d\tau d\eta \right\} \quad (3.8)$$

where $c_2(\alpha) = \sin((1 - \alpha/2)\pi)(c_1(\alpha)\pi)^{-1}$. and

$$k'(t) = \frac{1}{2}(w_t(0, t) - h'(t)) - \int_0^t D_{0+}^{2-\alpha} G(t - \tau) f(u(1, \tau)) d\tau. \quad (3.9)$$

Hence we can rewrite the above integral equation by interchanging the order of integration

$$\begin{aligned} f(h(t)) &= d(t) - c_2(\alpha) \int_0^t \frac{1}{(t - \tau)^{\alpha/2}} \left(\int_0^\tau G^{2-\alpha}(\tau - s) f(u(1, s)) ds \right) d\tau \\ &\quad - c_2(\alpha) \int_0^t \frac{1}{(t - \tau)^{\alpha/2}} \left(\int_0^\tau H^{2-\alpha}(\tau - s) f(h(s)) ds \right) d\tau \end{aligned} \quad (3.10)$$

where $d(t) = c_2(\alpha) \int_0^t \frac{w_t(0,\tau) - h'(\tau)}{2(t-\tau)^{\alpha/2}} d\tau$ is a known function, $G^{2-\alpha}(t) = (D_{0+}^{1-\alpha}G(t))_t \in C^\infty([0, \infty))$ and $H^{2-\alpha}(t) = (D_{0+}^{1-\alpha}H(t))_t \in C^\infty([0, \infty))$ (Equation (2.8)) with all orders of derivative vanishing at $t = 0$.

Now if f is of a fixed sign (corresponding to either a cooling or heating situation) then $f(h(t))$ and $f(u(1,t))$ also have this sign given our assumption that $h(t)$ is monotone. Then by setting $\tilde{f}(t) = f(h(t))$, we obtain

$$\begin{aligned} \tilde{f}(t) = & d(t) - c_2(\alpha) \int_0^t \frac{1}{(t-\tau)^{\alpha/2}} \left(\int_0^\tau G^{2-\alpha}(\tau-s) \tilde{f}(h^{-1}(u(1,s))) ds \right) d\tau \\ & - c_2(\alpha) \int_0^t \frac{1}{(t-\tau)^{\alpha/2}} \left(\int_0^\tau H^{2-\alpha}(\tau-s) \tilde{f}(s) ds \right) d\tau. \end{aligned} \quad (3.11)$$

We write this as

$$\tilde{f}(t) = \mathbf{T}[h, \tilde{f}](t) \quad (3.12)$$

and the integral equation (3.11) in the form

$$f = \mathbf{T}[h, \tilde{f}] = d(t) + \mathcal{A}\mathcal{F}_1[\tilde{f}] + \mathcal{A}\mathcal{F}_2[\mathbf{F}_h(\tilde{f})] \quad (3.13)$$

where $\mathcal{A}[f]$ is the Abel operator

$$\mathcal{A}[f] = \int_0^t \frac{f(\tau)}{(t-\tau)^{\alpha/2}} d\tau \quad (3.14)$$

and $\mathcal{F}_1[f]$ and $\mathcal{F}_2[f]$ denote the linear operators of the Volterra type

$$\mathcal{F}_1[f] = -c_2(\alpha) \int_0^t H^{(2-\alpha)}(t-\tau) f(\tau) d\tau \quad (3.15)$$

$$\mathcal{F}_2[f] = -c_2(\alpha) \int_0^t G^{(2-\alpha)}(t-\tau) f(\tau) d\tau. \quad (3.16)$$

Here \mathbf{F}_h denotes the nonlinear mapping

$$f \rightarrow f \circ h^{-1}(u(1, t))$$

and $u(1, t)$ is the solution of our direct problem.

Our goal is to show that assumptions can be made in order for \mathbf{T} to have a unique fixed point. We do this using a series of lemmas.

Assuming A0 – A3 hold, then the properties of G and H from Lemma 2.4.3 give the following results. We will skip the proof of these results since they are similar with [45], and the new kernel $\frac{1}{t^\alpha/2}$ is still integrable when $0 < \alpha < 1$.

Lemma 3.1.4 *If $\psi(\cdot)$ is Lipschitz continuous, and f_1 and f_2 are in $Lip[0, T]$, then for $i=1, 2$*

$$\|\mathcal{F}_i[\psi(f_1)] - \mathcal{F}_i[\psi(f_2)]\|_1 \leq c\alpha_i(t)\|f_1 - f_2\|_\infty$$

where $\alpha_i(t) = O(t)$ as $t \rightarrow 0^+$ and $\|\cdot\|_1 = |\cdot|_1 + |\cdot|_\infty$ is the norm for Lipschitz continuous functions and $|\cdot|_1$ the usual seminorm defined by

$$|f|_1 = \sup_{0 \leq t_1 < t_2 \leq T} \frac{|f(t_1) - f(t_2)|}{|t_1 - t_2|}.$$

Lemma 3.1.5 *Under the same conditions of f_1 , f_2 and ψ we have $\|\mathcal{A}[\psi(f_1)] - \mathcal{A}[\psi(f_2)]\|_{\mathcal{H}} \leq c\|f_1 - f_2\|_\infty$. In fact, the Abel integral operator maps functions in $C^\beta(0, T)$ into functions in $C^{\beta+1-\alpha/2}[0, T]$.*

Lemma 3.1.6 *If A0 – A3 hold, then the function $d(t) = \mathcal{A}[w_t(0, t) - h'(t)]$ lies in $\mathcal{H}[0, T]$.*

Lemma 3.1.7 *If f_1 and f_2 are Lipschitz functions of their independent variable,*

then the solution of

$$\begin{cases} \partial_t^\alpha u^{(i)} - u_{xx}^{(i)} = 0 & 0 < x < 1 \quad 0 < t < T \\ u^{(i)}(x, 0) = u_0(x) & 0 < x < 1 \\ u^{(i)}(0, t) = h(t) & 0 \leq t \leq T \\ u_x^{(i)}(1, t) = f_i(u^{(i)}(1, t)) = \tilde{f} \circ h^{-1}(u^{(i)}(1, t)) & 0 \leq t \leq T \end{cases} \quad (3.17)$$

for $i=1,2$, evaluated at $x = 1$ satisfies

$$\|u^{(1)}(1, t) - u^{(2)}(1, t)\|_{\mathcal{H}} \leq C \|\tilde{f}_1 - \tilde{f}_2\|_{\infty}$$

for T sufficiently small, and some constant C depending on T and the Lipschitz norms of f_1 and f_2 .

Theorem 3.1.1 *From Lemmas 3.1.4-3.1.7, we obtain $\mathbf{T} = \mathbf{T}[h, \cdot]$ is a contraction map on \mathcal{H} .*

In order to show that \mathbf{T} has a fixed point we require that the function $h^{-1}(u(1, t))$ be in the domain of \tilde{f} . In other words, we may only recover $f(u)$ over a range $U_0 \leq u \leq U_T$ if the overposed data $h(t)$ contains this set of values for $0 \leq t \leq T$. We thus require that $u(1, t)$ lies in the interval $[h(0), h(t)]$ for each t , $0 \leq t \leq T$. This will not hold in general. And hence we need the following assumption.

A4 For each t , $0 \leq t \leq T$, the function $u(1, t)$ lie in the interval $[h(0), h(t)]$.

In the case of (3.3) we can achieve this by taking more initial heat at the left end, which means taking u_0 decreasing in x . In the case of (3.4) we can obtain this by assuming that u_0 is constant and $g > 0$ or $g < 0$. Then we have

Theorem 3.1.2 *When $A0 - A4$ hold, \mathbf{T} has a unique fixed point on \mathcal{H} , i.e., there exists an unique solution to the inverse problem (3.1)-(3.5).*

Remark 3.1.1 *The monotonicity of $h(t)$, which is essential for the inversion step, will only hold under certain data inputs. These can be on the initial condition (for example, if u_0 is concave up) or on the flux input at the left boundary that should have a fixed sign (we are either cooling or heating). It is also possible to work the inverse problem piecewise according to the monotone intervals of $h(t)$. For example, if T_1, T_2, \dots denote the points where h changes monotonicity (and we assume there is only a finite number of these) then we can solve the inverse problem recursively on each subinterval. However, most physical situations that involve either a cooling or heating mode will not require this step.*

Remark 3.1.2 *Note the above representation as the solution of a nonlinear Volterra equation (or the equivalent fixed point argument) shows that we need only require h to be in C^1 . In fact, we really only need a fractional derivative assumption if $\alpha < 1$. In this situation the unique f is then continuous. Thus our inverse problem is only mildly ill-conditioned for $0 < \alpha \leq 1$; there is merely a derivative loss between the data function h and the recovered f (due to the presence of the term $h'(t)$). This assumption can be weakened further; if we rewrite the iteration scheme to include only $D^\alpha h$. This shows that the degree of ill-conditioning for the fractional diffusion equation is slightly less than the classical heat equation. However, it must be stated that such small differences are difficult to detect in practice.*

Remark 3.1.3 *This shows that any approach relying on analytically extending the Cauchy data on $x = 0$ to a solution u valid for $x = 1$, even if they were feasible in the case of $\alpha < 1$, would result in severe ill-conditioning. Such a solution $u(x, t)$ of the sideways heat conduction problem in the case of $\alpha = 1$ would not depend*

continuously on the Cauchy in any norm relying on a finite number of derivatives [7]. Attempting to recover f from the equation $u_x(1, t) = f(u(1, t))$ would only compound the difficulties.

3.2 Numerical examples

To obtain simulated data we used the direct solver described in Section 2.5.2 with a course grid (typically, $\Delta x = 0.02$ and $\Delta t = 0.01$) to obtain the value of $u(0, t)$ as the overposed data $\tilde{h}(t)$. We then added uniform noise of level σ to $\tilde{h}(t)$ at each grid point to obtain the data values $h_\sigma(t)$.

For the inverse problem we have two approaches based on our integral and differential interpretations: (3.11) and (3.20) (see below) respectively.

The first is in fact equivalent to the second but it has some computation drawbacks.

This approach requires the calculation of functions G and H in (3.11). We can just compute them initially and store them at the required grid points. Then we use (3.12) as $\tilde{f}_{n+1}(t) = \mathbf{T}[h, \tilde{f}_n](t)$ to iterate. This step requires integration with a weakly singular kernel and there are standard quadratures rules for this case. For example, in Section 4.4 of [51], we have the following formula to calculate improper integrals.

In fact, if the integrand $f(x)$ in the integration $\int_a^b f(x)dx$ diverges as $(x - a)^\gamma$ near $x = a$, where $0 \leq \gamma < 1$ (which is exactly our case), then we could make a change of variables and use the identity

$$\int_a^b f(x)dx = \frac{1}{1 - \gamma} \int_0^{(b-a)^{1-\gamma}} t^{\frac{\gamma}{1-\gamma}} f(t^{\frac{1}{1-\gamma}} + a)dt, \quad (b > a). \quad (3.18)$$

And if the singularity is at the upper limit, then we use the identity

$$\int_a^b f(x)dx = \frac{1}{1-\gamma} \int_0^{(b-a)^{1-\gamma}} t^{\frac{\gamma}{1-\gamma}} f(b - t^{\frac{1}{1-\gamma}})dt, \quad (b > a). \quad (3.19)$$

If there is a singularity at both limits, divide the integral at an interior breakpoint as above.

To compute G and H requires the evaluation of a Wright function, which is nontrivial. There are several means to accomplish this (see for example, [34]). To compute θ_α , we need infinite series and to achieve a high accuracy requires including a large number of terms, and each term is in itself a Wright function. Even in the classical case ($\alpha = 1$), computation of the kernel function $\theta(t)$ has similar difficulty when we have a much simpler function K included. Overall, this is a more computationally expensive option than the finite difference scheme. A finite difference scheme, for example Crank-Nicolson, is faster and can give us the same results under similar tolerances.

In what we show below we will use the second approach by performing the following steps.

- In order to avoid an 'Inverse Crime', we use a finer grid mesh to compute the forward solution to be used in the inverse problem ($\Delta x = 0.01$ and $\Delta t = 0.005$). Since there is still mild ill-conditioning we must regularize the solution and this is achieved in two stages. First, we obtain a function $h(t)$ from $h_\sigma(t)$ using a smoothing spline with parameters set to take into account the known value at $t = 0$ (through the compatibility condition) as well as the estimate of the noise level σ . We also take the opportunity to express h on a finer grid for use in steps below. Second, we take a basis representation of the unknown f , $f(u) = \sum_{k=1}^m c_k \phi_k(u)$ for given $\{\phi_n\}$ and coefficients $\{c_k\}$ that have to

be determined. In practice we used either a polynomial or a trigonometric basis. The number m of basis elements represents a further regularization of the problem. This step is not an essential factor in regularization which is primarily achieved through the smoothing spline, but it is a very convenient way to obtain values of the current approximation f at any given point.

- We make an initial approximation $f_0(u)$ and solve the following for $u_n(x, t)$, $n = 0, 1, \dots$:

$$\begin{cases} \partial_t^\alpha u = u_{xx}, & 0 < x < 1, 0 < t < T \\ u(x, 0) = u_0(x), & 0 < x < 1, \\ u(0, t) = h(t), & 0 < t < T, \\ -u_x(1, t) = f_n(u(1, t)), & 0 \leq t \leq T. \end{cases} \quad (3.20)$$

Evaluating u_n on $x = 0$ leads to the update equation $f_{n+1}(h(t)) := \frac{\partial}{\partial x} u_n(0, t)$ which we write as

$$f_{n+1}(z) := \frac{\partial}{\partial x} u_n(0, h^{-1}(z)). \quad (3.21)$$

From this we obtain the next iterate f_{n+1} . The value of $\frac{\partial}{\partial x} u_n(0, t)$ is calculated from a three points difference scheme.

- Equivalent to (3.12), we perform (3.20) and (3.21) and terminate when $\|f_n - f_{n+1}\|_{L^2}$ is obtained within a given accuracy.

As an alternative to the basis representation, at each stage when we solve (3.21) at a set of points $\{z_i\}$, $z_i = h(t_i)$ we could represent f again as set of spline coefficients. In addition this could be a smoothing spline and this would make the smoothing of the data h_σ less critical in the sense of exact choice of smoothing parameter. This would then transfer smoothing from the data onto the function f itself.

We present two examples to verify the procedure described above.

Example 3.2.1 *In this example, we solve the following problem:*

$$\begin{cases} \partial_t^\alpha u = u_{xx}, & 0 < x < 1, 0 < t < 1 \\ u(x, 0) = x^3, & 0 < x < 1, \\ u_x(0, t) = f(u(0, t)) + \beta_0(t), \quad -u_x(1, t) = f(u(1, t)) + \beta_1(t), & 0 \leq t \leq 1. \end{cases} \quad (3.22)$$

with exact values: $f(u) = 1 + u + u^2 + u^3 + u^4$, $\alpha = 0.5$ and the noise level $\sigma = 0.05$. Here $\beta_0(t)$ and $\beta_1(t)$ are chosen to make sure the compatibility condition is satisfied and the range of $u(0, t)$ contains that of $u(1, t)$ when $0 < t < 1$. We use the polynomial basis to represent f and the graph of approximated f_{app} and the exact f_{exact} are shown in Figure 3.1. We get a smaller than 4% relative error after only 5 iterations. We admit that this f can be written as the linear combination of our polynomial basis but include this example since both the Newton's law of cooling and the Stefan-Boltzmann law are polynomials with respect to u . Since these are common occasions, it is worthwhile to reconstruct $f(u)$ in polynomial form when we assume a combination of these two laws.

Example 3.2.2 *In this example, we solve the following problem*

$$\begin{cases} \partial_t^\alpha u = u_{xx}, & 0 < x < 1, 0 < t < 1 \\ u(x, 0) = -(x - 1/4)^2 + 4, & 0 < x < 1, \\ u_x(0, t) = f(u(0, t)) + \beta_0(t), \quad -u_x(1, t) = f(u(1, t)) + \beta_1(t), & 0 \leq t \leq 1. \end{cases} \quad (3.23)$$

with exact values: $f(u) = \frac{2}{1+20e^{-2u}}$, $\alpha = 0.5$ and the noise level $\sigma = 0.05$. Here $\beta_0(t)$ and $\beta_1(t)$ are chosen to ensure the compatibility and range conditions. We use

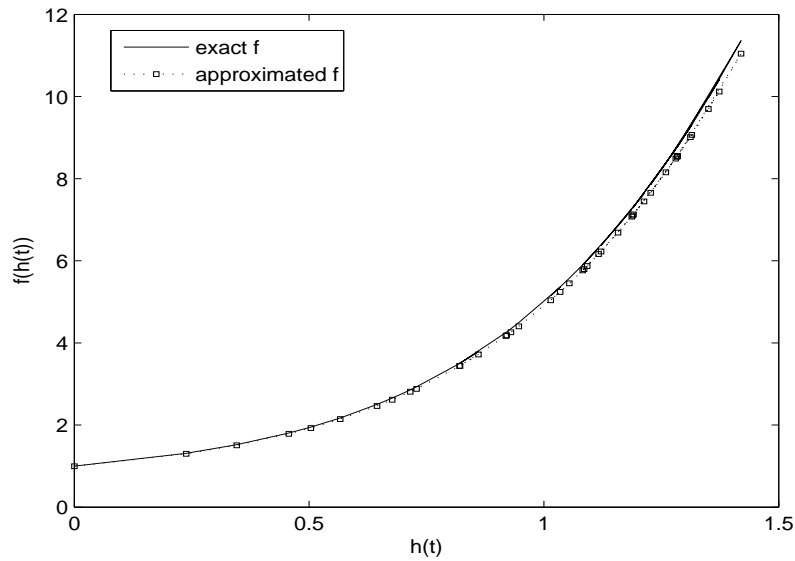


Figure 3.1: Example 3.2.1 Numerical $f(u)$ and exact $f(u)$

a trigonometric basis to represent f . The graph of approximated f_{app} and the exact f_{exact} are shown in Figure 3.2.

Suppose we do not know the exact value of α , how does this change the reconstruction? If its true value is $\alpha = 0.5$, but instead we use any of $\alpha = 0.51, 0.53, 0.55$ for the reconstruction stage, then as expected, the further α is from 0.5, the larger the error. However a relatively small error in α does not lead to dramatic differences for function f . The reconstruction results are shown in Figure 3.3.

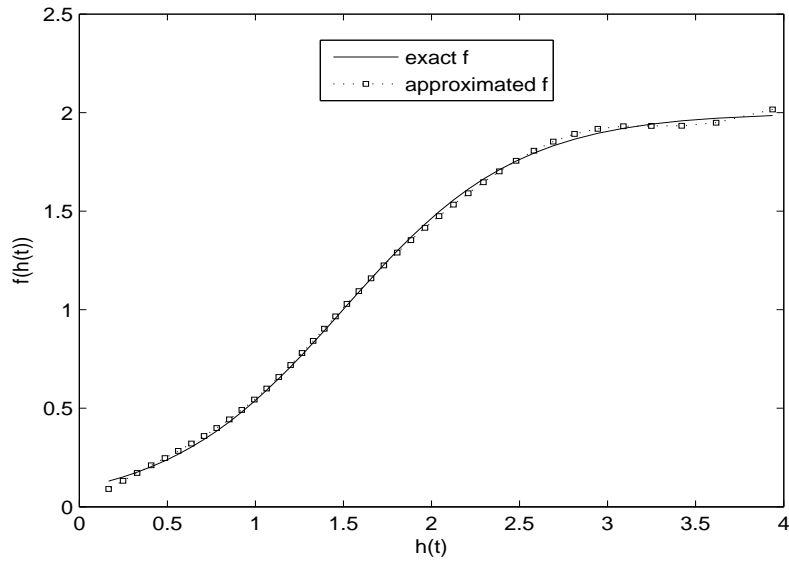


Figure 3.2: Example 3.2.2 Numerical $f(u)$ and exact $f(u)$

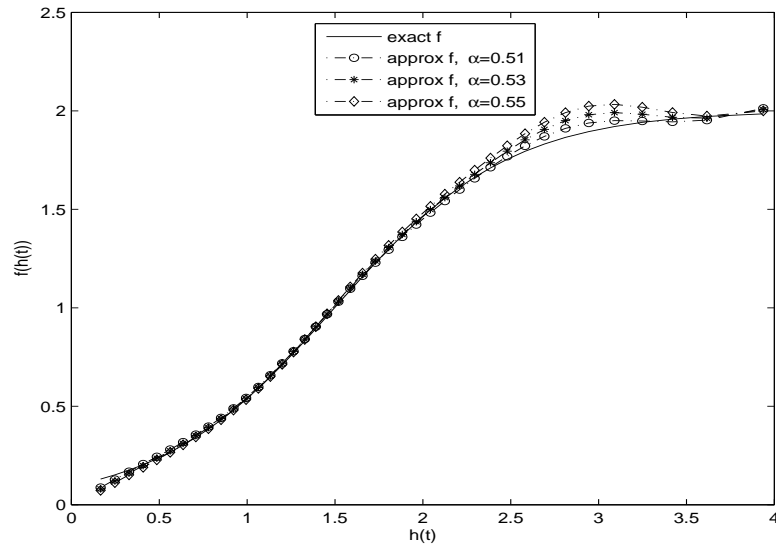


Figure 3.3: The role of α

4. INVERSE SOURCE PROBLEMS FOR ONE FRACTIONAL DIFFUSION EQUATION*

We consider an inverse problem for the time-fractional reaction-diffusion equation, which seeks to reconstruct the exact form of the unknown source f from the time trace of the solution at a fixed point x_0 under the assumption that f is a function that depends only on the state variable. The initial condition and the Neumann boundary condition are assumed to be given, and x_0 is located either in the interior or on the boundary $\partial\Omega$ of the domain Ω where the fractional reaction-diffusion equation is defined.

For the conventional reaction-diffusion equation, this is a classical problem that has been considered in e.g. [13] and [46], where uniqueness results and an iterative method for determination of the source function are presented.

The rest of this section is organized as follows. In Section 4.1, a uniqueness result for the problem under consideration is proved in the n -dimensional case and $x_0 \in \Omega$. The key of the proof is the maximum principle for the generalized time-fractional diffusion equation with the Caputo derivative that has been formulated and proved in Theorem 2.4.5. Section 4.2 is devoted to the case when $x_0 \in \partial\Omega$. Here we restrict ourselves to the one-dimensional case and use a different approach that allows us to represent the unknown source function f as a fixed point solution of an integral equation to show both uniqueness and existence of the solution. The existence of a unique fixed point is proved by means of the contraction mapping theorem and in a natural way provides an iterative procedure which by standard methods leads

*Portions of this section are reprinted with permission from "Uniqueness and reconstruction of an unknown semilinear term in a time-fractional reaction-diffusion equation" by Yuri Luchko, William Rundell, Masahiro Yamamoto and Lihua Zuo, 2013 Inverse Problems 29 065019 doi:10.1088/0266-5611/29/6/065019, Copyright [2013] by IOP.

to convergence estimates of the approximate solutions. Finally, in Section 4.3 a numerical example is presented to illustrate the validity of the proposed method.

4.1 Uniqueness results

In this section, we consider an initial-boundary-value problem with Neumann boundary conditions for the fractional reaction-diffusion equation in the form

$$\begin{cases} \partial_t^\alpha u(x, t) = \Delta u(x, t) + f(u(x, t)), & 0 < \alpha < 1, x \in \Omega, 0 < t < T, \\ \partial_\nu u(x, t) = g(x, t), & x \in \partial\Omega, 0 < t < T, \\ u(x, 0) = u_0, & x \in \Omega. \end{cases} \quad (4.1)$$

In (4.1), $\Omega \subset \mathbb{R}^n$ is a bounded domain with a smooth boundary $\partial\Omega$, $\nu(x) = (\nu_1(x), \dots, \nu_n(x))$ denotes the unit outward normal vector to $\partial\Omega$ at x , $\partial_\nu u = \nabla u \cdot \nu$, and the Caputo fractional derivative ∂_t^α of order α , $0 < \alpha < 1$ is defined by

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

We further assume that u_0 is a constant and $g(x, t) > 0$, $x \in \partial\Omega$ if $t > 0$ is sufficiently small. We are given the constant initial condition u_0 and the flux values $g(x, t)$ on $\partial\Omega$, but the source function $f(u)$ is unknown and has to be determined from the time trace at a fixed point $x_0 \in \bar{\Omega}$

$$u(x_0, t) = h(t). \quad (4.2)$$

For the problem (4.1), we assume existence of a solution $u = u(f) \in C(\bar{\Omega} \times [0, T])$, such that $u(x, \cdot) \in W^{1,1}(0, T)$ for $x \in \bar{\Omega}$ and $u(\cdot, t) \in C^2(\bar{\Omega})$ for $t > 0$ (for results regarding existence of solutions to nonlinear fractional differential equations with

the Caputo fractional derivative and their regularity properties we refer the reader to e.g. [11]).

In this section, we show uniqueness of a solution to the inverse problem formulated above under the condition that the source function f belongs to the space of functions \mathcal{F} defined by

$$\mathcal{F} = \{f \in C^1(\mathbb{R}) : f(r) > 0, r \in (u_0 - \varepsilon, u_0 + \varepsilon), \quad f'(r) < 0, r \in (u_0, u_0 + \varepsilon)\},$$

where $\varepsilon > 0$ is a constant.

First we prove the following auxiliary result.

Lemma 4.1.1 *Let $u(f_j)$ satisfy (4.1). There exists $\delta > 0$ such that*

$$u_1(x, t), u_2(x, t) > u_0, \quad x \in \overline{\Omega}, 0 < t \leq \delta.$$

Proof For $j = 1, 2$ we set $u(f_j) = u_j$. By $u_j \in C(\overline{\Omega} \times [0, T])$, for $\varepsilon > 0$, there exists $\delta_j > 0$ such that $u_0 - \varepsilon < u_j(x, t) < u_0 + \varepsilon$ for $x \in \overline{\Omega}$ and $0 \leq t \leq \delta_j$, and $g(x, t) > 0$ for $x \in \partial\Omega$ and $0 < t \leq \delta_j$. We put $\delta = \min\{\delta_1, \delta_2\}$, then

$$u_0 - \varepsilon < u_j(x, t) < u_0 + \varepsilon, \quad x \in \overline{\Omega}, 0 \leq t \leq \delta, \quad g(x, t) > 0, \quad x \in \partial\Omega, 0 < t \leq \delta. \tag{4.3}$$

We now prove

$$u_j(x, t) \geq u_0, \quad x \in \overline{\Omega}, 0 \leq t \leq \delta. \tag{4.4}$$

Assume that (4.4) does not hold. Then there exist $x_0 \in \overline{\Omega}$ and $t_0 \in [0, \delta]$ such that $u_j(x, t)$ attains the minimum $u_j(x_0, t_0) < u_0$ over $\overline{\Omega} \times [0, \delta]$. By $u_j(x, 0) = u_0$, $x \in \overline{\Omega}$,

we have $t_0 > 0$. The extremum principle of the Caputo derivative ([36]) yields

$$\partial_t^\alpha u_j(x_0, t_0) \leq 0. \quad (4.5)$$

Let $x_0 \in \partial\Omega$ and $u_j(x_0, t_0) < u_j(x, t_0)$ for all $x \in \Omega$. Then the strong maximum principle for Δ (e.g., Gilbarg and Trudinger [21]) implies

$$\partial_\nu u_j(x_0, t_0) < 0.$$

This is impossible by (4.3). Therefore we have the two possibilities: $x_0 \in \Omega$ and $x_0 \in \partial\Omega$ such that $u_j(x_0, t_0) \geq u_j(x_1, t_0)$ for some $x_1 \in \Omega$. For both cases, there exists some point in Ω denoted again by x_0 such that $u_j(x_0, t_0)$ is the minimum of $u_j(x, t)$ over $\bar{\Omega} \times [0, \delta]$. Therefore $\Delta u(x_0, t_0) \geq 0$ for both cases. Hence

$$f_j(u_j(x_0, t_0)) \leq \Delta u_j(x_0, t_0) + f_j(u_j(x_0, t_0)) = \partial_t^\alpha u_j(x_0, t_0) \leq 0$$

by (4.5). This is impossible by $f_j(u_j(x_0, t_0)) > 0$. Thus (4.4) follows.

Next we prove

$$u_j(x, t) > u_0, \quad x \in \bar{\Omega}, \quad 0 < t \leq \delta.$$

Assume that this does not hold. That is, there exist $x_0 \in \bar{\Omega}$ and $0 < t_0 \leq \delta$ such that $u_j(x_0, t_0) = u_0$. By (4.4), u_0 is the minimum of $u_j(x, t)$, $(x, t) \in \bar{\Omega} \times [0, \delta]$ and so we repeat the previous argument to reach a contradiction. Thus the proof of Lemma 4.1.1 is completed. ■

We show the local uniqueness within a sub-class of \mathcal{F} satisfying the finitely many crossing condition.

Theorem 4.1.1 *Let $f_1(r)$ and $f_2(r)$ be such that on any interval $[u_0, u_*]$ of finite length, there are at most finitely many isolated zeros of $f_1 - f_2$. If*

$$u(f_1)(x_0, t) = u(f_2)(x_0, t) \quad \text{for some } x_0 \in \overline{\Omega} \text{ and } 0 \leq t \leq T, \quad (4.6)$$

then there exists $0 < \varepsilon_0$ such that $f_1(r) = f_2(r)$ for $u_0 \leq r \leq u_0 + \varepsilon_0$.

Proof Assume that the conclusion is not true. That is, there exists $\varepsilon_1 > 0$ such that $0 < \varepsilon_1 < \varepsilon$ and

$$f_1(r) \neq f_2(r), \quad u_0 < r < u_0 + \varepsilon_1.$$

We note that $f_1(u_0) = f_2(u_0)$ may hold. Without loss of generality, we can assume that

$$f_1(r) > f_2(r), \quad u_0 < r \leq u_0 + \varepsilon_1. \quad (4.7)$$

On the other hand, $f_1(u_1) - f_2(u_2)$ can be represented in the form

$$f_1(u_1) - f_2(u_2) = f_1(u_1) - f_1(u_2) + f_1(u_2) - f_2(u_2) = f_1'(z)u + f_1(u_2) - f_2(u_2)$$

with $z = u_2 + \theta u$, $0 < \theta < 1$ and u satisfies the equations

$$\begin{cases} \partial_t^\alpha u(x, t) = \Delta u(x, t) + f_1'(z)u + f_1(u_2) - f_2(u_2), & x \in \Omega, 0 < t < T, \\ \partial_\nu u(x, t) = 0, & x \in \partial\Omega, 0 < t < T, \\ u(x, 0) = 0, & x \in \Omega. \end{cases}$$

Hence by (4.3) and Lemma 4.1.1, choosing $\delta > 0$ small again if necessary, we see that $u_0 < u_2(x, t) < u_0 + \varepsilon_1$ for $x \in \overline{\Omega}$ and $0 < t \leq \delta$, and so (4.7) yields

$$f_1(u_2(x, t)) - f_2(u_2(x, t)) > 0 \quad (4.8)$$

for $x \in \overline{\Omega}$, $0 < t \leq \delta$.

We prove

$$u(x, t) \geq 0, \quad x \in \overline{\Omega}, 0 \leq t \leq \delta. \quad (4.9)$$

Assume that (4.9) is not true. Then there exists $(x_0, t_0) \in \overline{\Omega} \times [0, \delta]$ such that u attains the minimum $u(x_0, t_0) < 0$. By the initial condition, we conclude that $t_0 > 0$.

Therefore the extremum principle of the Caputo derivative ([36]) yields

$$\partial_t^\alpha u(x_0, t_0) \leq 0.$$

Let $x_0 \in \partial\Omega$. Therefore by $\partial_\nu u(x_0, t_0) = 0$ and $u(x_0, t_0)$ is the minimum of u , we have $\Delta u(x_0, t_0) \geq 0$. Also for the case of $x_0 \in \Omega$, we have $\Delta u(x_0, t_0) \geq 0$. There the equation in u , $u(x_0, t_0) < 0$ and $f_1'(z) \leq 0$ yield

$$\begin{aligned} 0 &\geq \partial_t^\alpha u(x_0, t_0) = \Delta u(x_0, t_0) + f_1'(z)u(x_0, t_0) + f_1(u_2(x_0, t_0)) - f_2(u_2(x_0, t_0)) \\ &\geq f_1(u_2(x_0, t_0)) - f_2(u_2(x_0, t_0)), \end{aligned}$$

which is impossible by (4.8). Thus (4.9) is proved.

Next we prove

$$u(x, t) > 0, \quad x \in \overline{\Omega}, 0 < t \leq \delta. \quad (4.10)$$

Assume that this does not hold, that is, there exist $x_0 \in \overline{\Omega}$ and $0 < t_0 \leq \delta$ such that $u(x, t)$ attains the minimum 0 over $\overline{\Omega} \times [0, \delta]$. Repeating the previous argument, we reach a contradiction, and the proof of (4.10) is completed. The inequality (4.10) contradicts (4.6) and so the proof of Theorem 4.1.1 is completed. \blacksquare

The global uniqueness results for the inverse problem under consideration can be derived from Theorem 4.1.1 under some additional conditions posed on the class of

functions \mathcal{F} that the source functions f have to belong to.

Corollary 2.1 *Let $f_1, f_2 \in \mathcal{F}$ be analytic functions. Then (4.5) implies $f_1 \equiv f_2$ on the whole \mathbb{R} .*

4.2 Existence results in the one-dimensional case

In this section, we restrict ourselves to the case of a single spatial variable. This certainly simplifies the analysis and leads to a clear understanding of the ideas. That is a primary goal in this problem. We expect that in analogy to the known results for the parabolic type PDEs ($\alpha = 1$), the extension of our method to the case of several spatial variables, although not routine and involving several technical issues above the single pspace varaible case, should also be possible.

Let Lip_1 denote the space of all uniformly Lipschitz continuous functions in the interval $[0, \infty)$. By $\|f\|_1$ we denote the Lipschitz constant of $f \in \text{Lip}_1$. We set

$$S = \{f : f \in \text{Lip}_1, \|f\|_1 \leq C_1\}$$

with arbitrarily fixed $C_1 > 0$.

Let $u(x, t)$ satisfy the fractional reaction-diffusion equation and the initial and boundary conditions in the form of

$$\begin{cases} \partial_t^\alpha u - u_{xx} = f(u) + \gamma(x, t), & 0 < x < 1, \quad 0 < t < T, \\ u(x, 0) = u_0(x), & 0 < x < 1, \\ u_x(0, t) = g_1(t), \quad -u_x(1, t) = g_2(t), & 0 \leq t \leq T, \end{cases} \quad (4.11)$$

with overposed data

$$u(0, t) = h(t), \quad 0 \leq t \leq T. \quad (4.12)$$

In (4.11), $u_0(x)$, $g_1(t)$, $g_2(t)$, and $\gamma(x, t)$ are given functions that fulfill the conditions

formulated below, and ∂_t^α is the Caputo fractional derivative of order α , $0 < \alpha < 1$.

The problem is to recover the nonlinear reaction function f from the measured overposed data $h(t)$. The function $f(u)$ depending on u can be only determined on the range of states actually reached. In the general case, this is usually unknown as it depends on f . However, if we force the measurement (in this case $h(t)$) to contain the entire range of $u(x, t)$ on the whole domain, then that range is known. Conditions below are chosen to ensure this. They are sufficient but certainly not necessary. Other combinations could also achieve the same end, as we will demonstrate by an example later.

- **A1.** f belongs to the space S .
- **A2.** $\gamma_x \leq 0$ belongs to the space $C^1([0, 1] \times [0, T])$.
- **A3.** $u_0(x)$ is a constant.
- **A4.** g_i ($i = 1, 2$) belongs to the space $C^1[0, T]$ and $g_2(t) < -g_1(t)$ for $0 \leq t \leq T$.

Remark 4.2.1 *The conditions **A2**, **A3** and **A4** on functions γ_x , u_0 , g_1 and g_2 are imposed to ensure that the maximum range of $u(x, t)$ is at the line $x = 0$. By **A3** and **A4**, the profile of $u(x, t)$ starts from a constant and gets more heat on the left hand side than the right hand side, so the temperature increases faster on the left hand side.*

We now introduce the auxiliary functions K and ψ given by

$$K(x, \xi, t - \tau) = (D_{0+}^{1-\alpha} \theta_\alpha)(x - \xi, t - \tau) + (D_{0+}^{1-\alpha} \theta_\alpha) \theta_\alpha(x + \xi, t - \tau) \quad (4.13)$$

$$\psi = w + v_1 + v_2 + \int_0^t \int_0^1 K(x, \xi, t - \tau) \gamma(\xi, \tau) d\xi d\tau. \quad (4.14)$$

Then by Lemma 2.4.6, the solution u to the problem (4.11) can be rewritten in the form

$$u(x, t) = \psi + \int_0^t \int_0^1 K(x, \xi, t - \tau) f(u(\xi, \tau)) d\xi d\tau. \quad (4.15)$$

For a given $f \in S$, let $u = u(x, t; f)$ be a solution to the problem (2.41) we define a mapping \mathbf{T} by the formula

$$\mathbf{T}[f] = \partial_t^\alpha h(t) - u_{xx}(0, t; f) - \gamma(0, t). \quad (4.16)$$

Remark 4.2.2 *The Assumptions A1-A4 ensure that $u_{xx}(0, t; f)$ is well-defined. In fact, for a given f , $u(x, t; f)$ can be computed since we know all values of f that the computation of u requires.*

Then we have the following important result:

Lemma 4.2.1 *Given $f \in S$, a function u is a solution to the problem (4.11) if and only if the function f is a fixed point of the mapping \mathbf{T} defined by (4.16).*

Proof If u is a solution of (4.11) with a function $f \in S$, then

$$\begin{aligned} f(h(t)) &= f(u(0, t)) \\ &= \partial_t^\alpha u(0, t) - u_{xx}(0, t) - \gamma(0, t) \\ &= \partial_t^\alpha h(t) - u_{xx}(0, t; f) - \gamma(0, t) = \mathbf{T}[f] \end{aligned}$$

and f is a fixed point of the mapping \mathbf{T} .

On the other hand, if f is a fixed point of the mapping \mathbf{T} , then we use the formula

$$\mathbf{T}[f] = \partial_t^\alpha h(t) - \partial_t^\alpha u(0, t) + f(u(0, t))$$

to conclude that

$$f(h(t)) = \partial_t^\alpha h(t) - \partial_t^\alpha u(0, t) + f(u(0, t)).$$

Introducing an auxiliary function $\delta(t) := u(0, t) - h(t)$, we get the relation

$$\partial_t^\alpha \delta(t) = \partial_t^\alpha u(0, t) - \partial_t^\alpha h(t) = f(u(0, t)) - f(h(t)).$$

Since $f \in S$, it follows that

$$|\partial_t^\alpha \delta(t)| \leq C_1 |\delta(t)|.$$

Because $\delta(0) = 0$, the Gronwall inequality for the Caputo fractional derivative (Lemma 4.3 in [12]) ensures that $\delta(t) = 0$ for $t > 0$, so that $u(x, t)$ satisfies (4.11). ■

Combining formulas (4.15) and (4.16), we get the representation

$$\mathbf{T}[f] = \partial_t^\alpha h(t) - \gamma(0, t) - \psi_{xx} - \int_0^t \int_0^1 K_{xx}(0, \xi, t - \tau) f(u) d\xi d\tau \quad (4.17)$$

for the mapping \mathbf{T} .

Since we have freedom to modify the constant C_1 if necessary, we can assume the condition $\|\partial_t^\alpha h - \gamma(0, t)\|_1 < \frac{1}{2}C_1$ on $[0, T_1]$. A solution $u(x, t)$ of (4.11) satisfies the equation

$$\begin{aligned} u(x, t) &= \psi + \int_0^t \int_0^1 K(x, \xi, t - \tau) f(u(\xi, \tau)) d\xi d\tau \\ &= \psi + \int_0^t \int_0^1 K(x, \xi, t - \tau) \omega(\xi, \tau; f, u) u(\xi, \tau) d\xi d\tau, \end{aligned}$$

where $\omega = \frac{f(u)}{u}$ is an L_∞ function bounded by the constant C_1 since $f \in S$.

Solving this equation for u , we get the formula

$$u(x, t) = \psi + \int_0^t \int_0^1 \tilde{K}(0, \xi, t - \tau) \psi(\xi, \tau) d\xi d\tau, \quad (4.18)$$

where \tilde{K} is the resolvent kernel for the integral equation with the kernel $K\omega$ given above. It follows from the Neumann expansion of the Volterra integral equations that the kernels K and \tilde{K} have the same regularity properties.

By Lemma 2.4.4, $\lim_{t \rightarrow 0} \tilde{K}_{xx}(x, t) = 0$, so that \tilde{K}_{xx} is continuous and bounded on $[0, t] \times [0, 1]$, thus $\exists A > 0$, such that $|\tilde{K}_{xx}(0, \xi, t - \tau)| < A$ for $0 \leq \tau \leq t$ and $0 \leq x \leq 1$ and. Then the estimate

$$\left\| \int_0^t \int_0^1 \tilde{K}_{xx}(0, \xi, t - \tau) \psi(\xi, \tau) d\xi d\tau \right\|_1 \leq A \|\psi\|_1 \quad (4.19)$$

holds uniformly in time for $0 \leq t \leq T$, where A is an absolute constant.

From the formulas (4.18) and (4.19) and the fact that $|\psi_{xx}(0, t)| = |\partial_t^\alpha h(t) - \gamma(0, t)|$ can be chosen to be bounded and $\psi_{xx}(x, t)$ is continuous with respect to x ,

$$\|u_{xx}\|_1 \leq \|\psi_{xx}\|_1 + A\|\psi\|_1.$$

The right-hand side of this inequality can be made smaller than $\frac{1}{2}C_1$ by choosing a sufficiently small time interval $[0, T_2]$. In this case, we get

$$\|u_{xx}\|_1 < \frac{1}{2}C_1.$$

Combining both inequalities, we have

$$\|\mathbf{T}[f]\|_1 \leq \|\partial_t^\alpha h - \gamma\|_1 + \|u_{xx}\|_1 < C_1$$

for $0 < t < T^*$, $T^* = \min\{T_1, T_2\}$ that means that the mapping \mathbf{T} is bounded in S . We now show that the Gateaux derivative of \mathbf{T} vanishes at $t = 0$. Indeed, the relation

$$\mathbf{T}[f + s\theta] = \partial_t^\alpha h - u_{xx}^s(0, t; f + s\theta) - \gamma(0, t)$$

holds, where $u^s = u(x, t; f + s\theta)$ satisfies the equation

$$\partial_t^\alpha u^s - u_{xx}^s = f(u^s) + s\theta(u^s) + \gamma(x, t).$$

Differentiating this with respect to s and letting $s = 0$, we get the relation

$$\hat{\mathbf{T}} := \mathbf{T}'[f] \cdot \theta = \hat{u}_{xx}(0),$$

where $\hat{u} = \frac{du^s}{ds}|_{s=0}$ satisfies the equation

$$\partial_t^\alpha \hat{u} - \hat{u}_{xx} = f'(u)\hat{u} + \theta(u)$$

with homogeneous initial and boundary conditions. Solving this equation for \hat{u} , we get

$$\hat{u} = \int_0^t \int_0^1 \hat{G} \theta(u) d\xi d\tau,$$

where \hat{G} is the fundamental solution to the fractional diffusion equation with an L_∞ coefficient in $\partial_t^\alpha v - v_{xx} - f'(u)v = 0$ that satisfies homogeneous Neumann boundary

conditions. Then the inequalities

$$\|\hat{u}_{xx}\|_\beta \leq CA\|\theta\|_\beta \leq Ct^{1-\beta}\|\theta\|_1 \quad (4.20)$$

with a generic constant C follow from (4.19) for any $0 < \beta < 1$. Here $\|u\|_\beta$ is the Hölder norm defined as

$$\|\theta\|_\beta = \max_{u \in \Omega} |\theta(u)| + \sup_{u, v \in \Omega, u \neq v} \frac{|\theta(u) - \theta(v)|}{|u - v|^\beta},$$

where Ω is the domain, so that the last inequality holds with $t^{1-\beta}$ by the Compact Embedding Theorem 1.1.1 between Hölder spaces C^β and C^1 . Since $\|\hat{\mathbf{T}}\|_\beta = \|\hat{u}_{xx}\|_\beta$ and $\theta \in S$, we obtain the inequality $\|\hat{\mathbf{T}}\|_\beta \leq Ct^{1-\beta}$. Thus the Gateaux derivative $\hat{\mathbf{T}}$ vanishes at the origin that means that for small enough values of t , say for $t < T^*$, the norm of $\hat{\mathbf{T}}$ is less than unity. Therefore, the mapping \mathbf{T} is a contraction on C^β for $0 < \beta < 1$.

Remark 4.2.3 *Inequality (4.20) can be proved under higher regularity assumptions on f and θ . Then we need to show that the mapping \mathbf{T} still maps this new space of f to itself, which will complicate the proof in the previous part. It is reasonable to conjecture that this inequality also holds under our assumptions. This will be worked out in the future. This regularity requirement won't be an issue for the numerical simulation, because we just need to project f to the space we want. As we will see in the next section, this is easily achieved since we use a smooth basis set to expand f .*

We thus have proved the following result:

Lemma 4.2.2 *The mapping \mathbf{T} possesses a unique fixed point on S when $t < T^*$, i.e., the inverse problem (4.11) has a unique solution on the range $[h(0), h(T^*)]$.*

When $t > T^*$, let $q(x) = u(x, T^*)$ and $\varphi(x, t) := u(x, t) - u(x, T^*)$, so that φ satisfies the relations

$$\begin{cases} \partial_t^\alpha \varphi - \varphi_{xx} = f(\varphi + q(x)) + \gamma(x, t) + q_{xx}(x), \\ \varphi(x, T^*) = 0, \\ \varphi_x(0, t) = g_1(t) - g_1(T^*) := \tilde{g}_1(t), \\ -\varphi_x(1, t) = g_2(t) - g_2(T^*) := \tilde{g}_2(t). \end{cases}$$

Once again, we define a mapping as follows:

$$\mathbf{T}[f] = \partial_t^\alpha h(t) - \varphi_{xx}(0, t) - q_{xx}(0) - \gamma(0, t).$$

When we define a comparison function ψ that satisfies the equation

$$\partial_t^\alpha \psi - \psi_{xx} = \gamma(x, t) + q_{xx}(x)$$

with the same initial and boundary conditions as φ , the mapping \mathbf{T} can be represented in the form

$$\mathbf{T}[f] = \partial_t^\alpha h(t) - \partial_t^\alpha \psi(0, t) + \psi_{xx}(0, t) - \varphi_{xx}(0, t).$$

To guarantee an extension of the result formulated in Lemma 4.2.2 to the case $t > T^*$ it is sufficient to verify the inequalities

$$\|\partial_t^\alpha h(t) - \partial_t^\alpha \psi(0, t)\|_1 < 1/2C_1,$$

$$\|\psi_{xx}(0, t) - \varphi_{xx}(0, t)\|_1 < 1/2C_1$$

These hold since the quantities inside the norms vanish at $t = T^*$. Summarizing the results formulated in the previous lemmas we thus proved the following main theorem.

Theorem 4.2.1 *The inverse problem of determining a nonlinear reaction function in (4.11) has a unique solution under the assumptions **A1–A4**.*

Remark 4.2.4 *It should be noted that the unknown source function f in the inverse problem which we considered in this section, is determined as the unique solution of a nonlinear Volterra integral equation which follows from the representation formulas in the proofs of the lemmas. The assumptions posed on the class of the source functions f is one sufficient condition for unique existence of solution to this inverse problem, and there may be other sufficient conditions.*

Remark 4.2.5 *Since the mapping \mathbf{T} defined in (4.17) is a contraction, the convergence rate of successive iterates can be obtained through the routine technique of computing the convergent Neumann expansion of the associate Volterra equation.*

4.3 Numerical example of reconstruction of the unknown source function

To generate the overposed data $h(t)$, a direct solver for the nonlinear fractional diffusion equations is needed. In our numerical example, we used the finite difference scheme described in Section 2.5.2 with some modifications to include the nonlinear source term.

The direct solver produces the overposed data $\tilde{h}(t)$ as the values of $u(0, t)$. To test our reconstruction method, uniform noise of level σ was added to $\tilde{h}(t)$ at each grid point that resulted in the the data values denoted by $h_\sigma(t)$.

Our reconstruction algorithm consists of the following steps:

- Since the algorithm requires computing a fractional derivative of $h_\sigma(t)$, and this is (mildly) ill-conditioned, we regularize this function at the outset by using a smoothing spline with parameters set that takes into account the known noise level σ and the known compatibility condition at $t = 0$. The resulting function is then interpolated on a finer grid for use in the next steps.
- A representation of the unknown function f in a basis ϕ_k , $k \in \mathbb{N}$ in the form $f(u) = \sum_{k=1}^m c_k \phi_k(u)$ is introduced, where the coefficients c_k , $k \in \mathbb{N}$ have to be determined. Theoretically, an arbitrary basis can be used, but in practice, and is as usual in inverse problems, a priori information regarding the possible form of f is important for the choice of selecting the basis. For example, both Newton's and Stefan-Boltzmann's laws assume a power law for f . If our model indicates that f follows Newton's law for low temperatures and Stefan-Boltzmann's law for high temperatures, then a basis of smooth functions may be reasonable, perhaps just the polynomial basis as a potential interpolant between the two regimes. If we suspect there exists a phase change, then a piecewise linear basis may be preferable. When we have no such information available other than that f should be smooth, then a trigonometric basis (modified for possible endpoint constraints) might be a good choice.

To proceed with the inverse problem algorithm, an initial approximation for $f_0(u)$ is made and the direct problem

$$\begin{cases} \partial_t^\alpha u - u_{xx} = f_n(u) + \gamma(x, t), & 0 < x < 1, 0 < t < T \\ u(x, 0) = u_0(x), & 0 < x < 1, \\ u_x(0, t) = g_1(t), & 0 < t < T, \\ -u_x(1, t) = g_2(t), & 0 \leq t \leq T \end{cases}$$

is solved for $u_n(x, t)$, $n = 0, 1, \dots$. Evaluating u_n at the point $x = 0$ (this value is then denoted by $h_n(t)$) leads to the updated equation

$$\partial_t^\alpha h(t) - u_{xx}(0, t; f_n) = f_{n+1}(h) + \gamma(0, t) \quad (4.21)$$

which is equivalent to the mapping \mathbf{T} introduced in the previous section. The value of $u_{xx}(0, t)$ is calculated based on a four points difference scheme. The value of f_{n+1} is obtained by solving the equation (4.21). In fact, since $f_{n+1}(h) = \sum_{k=1}^m c_k^{n+1} \phi_k(h)$, we just need to solve for the coefficients c_k^{n+1} the linear system

$$\sum_{k=1}^m c_k^{n+1} \phi_k(h) = \partial_t^\alpha h(t) - \gamma(0, t).$$

- The above iteration process is terminated when the inequality $\|f_n - f_{n+1}\|_{L^2} < \varepsilon$ is fulfilled with a given accuracy ε .

In the first numerical example, we show what will happen if the range condition mentioned in Remark (4.2.2) failed.

Example 4.3.1

$$\begin{cases} \partial_t^\alpha u - u_{xx} = f(u) + \gamma(x, t), & 0 < x < 1, 0 < t < 1 \\ u(x, 0) = 0, & 0 < x < 1, \\ u_x(0, t) = -t, \quad -u_x(1, t) = t^2, & 0 \leq t \leq 1. \end{cases} \quad (4.22)$$

In (4.3.1) we took $\alpha = 0.5$ and the nonlinear source term f that has to be reconstructed has the form $f(u) = -u^2 - u$. The Neumann boundary conditions are chosen to make the temperature range when $x = 0$ is $[0, 0.5938]$, which is smaller than the range of $u(x, t)$, $[-0.1612, 0.5938]$, thus the range condition is not satisfied.

We use different first guesses $f_0 = 0$, $f_0 = 0.1$ and $f_0 = -1$ to start the iteration steps. The iteration results are shown in Figure 4.1. We can see that instead of converging to the same result as what we see in the case when the range condition is satisfied, different first guesses will generate vastly different result.

Remark 4.3.1 When we use first guess $f_0 > 0.2$, it starts to blow up after the second iteration, which is the reason why we used $f_0 = 0.1$ as our maximum first guess.

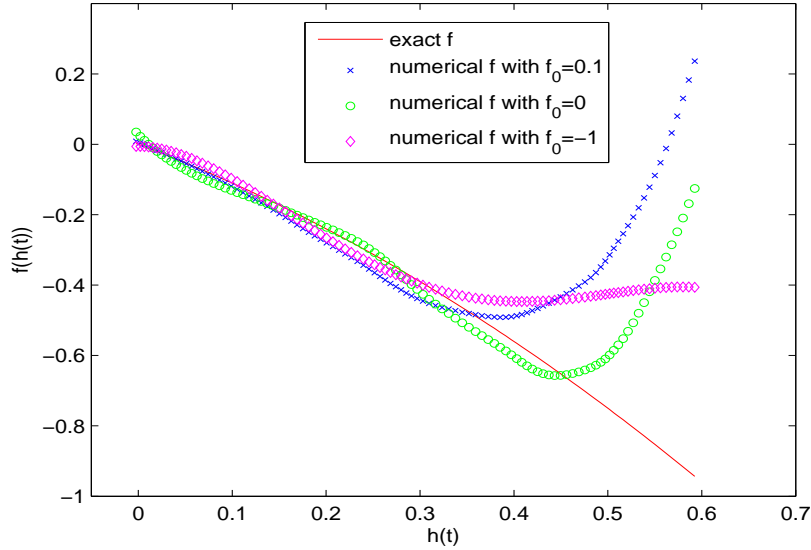


Figure 4.1: Example 4.3.1 Exact f and numerical f with different first guesses

Example 4.3.2 Consider the inverse problem in the form

$$\begin{cases} \partial_t^\alpha u - u_{xx} = f(u) + \gamma(x, t), & 0 < x < 1, 0 < t < 1 \\ u(x, 0) = \frac{1}{2}x^2, & 0 < x < 1, \\ u_x(0, t) = -t^2, \quad -u_x(1, t) = t^2 - 1, & 0 \leq t \leq 1. \end{cases} \quad (4.23)$$

In (4.3.2) we took $\alpha = 0.5$ and the nonlinear source term f that has to be reconstructed has the form $f(u) = -10(3u^2 - 2u^3)e^{-u}$. The function $\gamma(x, t)$ is chosen to satisfy the equation for the exact solution $u(x, t) = \frac{1}{2}x^2 + (1 - x)t^2$.

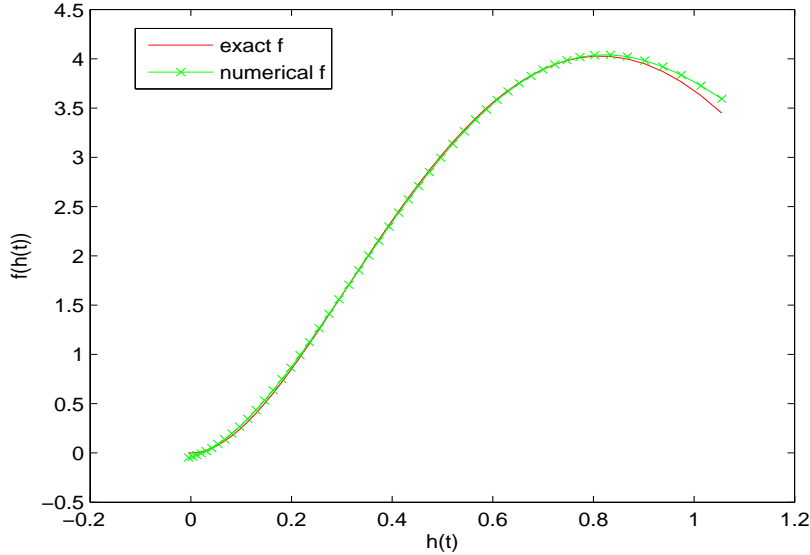


Figure 4.2: Example 4.3.2 Numerical f and exact f

The plots of the reconstructed source function f_{app} found with our algorithm and of the exact f_{exact} are shown in Figure 4.2. For the calculations, a polynomial basis was used (note that f_{exact} cannot be represented as a finite combination of the basis elements). The level σ of noise was chosen to be equal to 5%. Effective numerical convergence was achieved after 10 iterations starting even from the initial value $f_0 = 0$, which is a poor first guess. The results of relative errors for the actual coefficients c_k and computed coefficients c_k^n is shown in the table below.

Remark 4.3.2 *In this example, u_0 was chosen not to be a constant. We can compute that the condition $\gamma_x \leq 0$ also fails. This illustrates that the assumptions **A1-A4** are sufficient rather than necessary.*

Remark 4.3.3 *As we mentioned in Remark 4.2.2, the range condition which requires $\text{Range}\{u(x,t)(0 \leq x, t \leq 1)\} \subset \text{Range}\{h(t)(0 \leq t \leq 1)\}$, is essential for our iteration process. In Example 4.3.2, since the range condition is satisfied, we will have a converging iteration unless we choose a very bad first approximation.*

But if we do choose a bad first guess f_0 , which is possible if the exact $f(u) < 0$ but we use a $f_0 \gg 0$. Then even if the range condition is satisfied in the original problem, during the iterations, $f(u)$ may still need to call for values outside $h(t)(0 \leq t \leq 1)$. That will cause the same phenomena as in Example 4.3.1, which means different first guesses will lead to different iteration results.

To deal with this issue, we need to use some nonlocal basis that could 'extend' our $f(u)$. There are two choices we have, the polynomial basis and the trigonometric basis but not any compact supported basis. If we conjecture that either polynomial basis or trigonometric basis could approximate $f(u)$ properly, then we could use them to express the unknown $f(u)$ and extend the function $f(u)$ to the values beyond the range of h . Therefore we can continue our iterations by only passing the coefficients of f to the following iteration step, in which way $f(u)$ is easily extended globally.

There are two risks of the this analytical extension. The first is that once we use a large number of polynomial basis functions, the condition number of the corresponding Vandermonde matrix increases quickly. For example, if we only use 10 basis functions as the basis, the condition number is already $O(10^{12})$. The second risk is that if our conjecture is wrong, the extension could be totally different with the exact $f(u)$. To resolve this, we need to control the ill-conditionedness by restricting the numbers of the polynomial basis functions to be small.

As can be seen in Figure 4.2, the reconstructed source function f_{app} begins to differ from f_{exact} for large values of u . This is a direct consequence of the fact

Table 4.1: Relative errors between the correct coefficients and the approximated

$\delta_n \backslash n$	1	2	3	4	5	6	...	10	...	15
1	20.140	19.160	6.540	-1.060	-1.850	-0.900	...	1.810	...	2.450
u	-0.103	0.837	-4.320	-3.863	-2.092	-1.030	...	0.051	...	0.186
u^2	0.688	-0.035	0.585	0.527	0.280	0.141	...	0.013	...	0.001
u^3	0.670	-0.477	0.431	0.602	0.357	0.197	...	0.041	...	0.029
u^4	0.667	-1.268	-0.023	0.631	0.428	0.245	...	0.066	...	0.068

that in this example larger values of u correspond to larger times. According to Remark 4.2.4, approximation errors are accumulated from previous steps in the time-marching required for Volterra equations.

In Table 4.1, we can see from the relative errors $\delta_n := \frac{c_k - c_k^n}{c_k}$ between the correct coefficients and the approximated coefficients that the coefficients begin to diverge with large number of iterations n . This can be explained by the mild ill-conditioning of the fractional derivative and the fact that we haven't done any regularization during the calculations. Such regularization could be achieved by a variety of methods, although simply restricting the numbers of the basis functions and terminating the iteration early (using a stopping condition) suffices in most cases due to the mild level of ill-conditioning.

5. NUMERICAL METHOD FOR RECONSTRUCTING A SEMILINEAR TERM FROM INPUT SOURCES

In this section, our goal is to reconstruct the nonlinear source $Q(u)$ in the following problem:

$$u_t - u_{xx} = Q(u) + f_j(x, t) \quad 0 < x < 1, \quad 0 < t < T, \quad (5.1)$$

with homogenous Dirichlet boundary condition and zero initial condition by overposed data $\gamma_j = u_x^j(1, \bar{t}) - u_x^j(0, \bar{t})$ where \bar{t} is a certain time in $[0, 1]$ and u_j is the solution to the above equation corresponding to $f_j(x, t)$, $j = 1, \dots, N$.

5.1 Introduction

In most diffusion processes or heat transfer problems, linear equations are accurate enough to be a model for the underlying physical system. However, as we showed in Section 4, in many technical and industrial applications, in particular for large ranges of temperatures, nonlinear effects, which may be due to temperature dependence of material parameters or radiation, have to be considered. Nonlinear heat transfer laws appear, e.g., in the modeling of cooling processes for steel or glass in liquids and gases, e.g., in the continuous casting of steel ([23]), where they may obey the Stefan-Boltzmann law $f(u) = b(u^4 - u_0^4)$. Nonlinear diffusion equations also arise in furnace reactions (see [55]).

Prominent examples for inverse problems for diffusion equations are backwards or sideways heat equation, and a variety of parameter identification problems (for an account of some important inverse problems in diffusion see the Proceedings [19], or Beck, Blackwell and Clair [5] and Alifanov [4] for an overview over inverse heat conduction problems). Note, as we showed in Section 2.3.1, most of these inverse

problems are ill-posed, i.e. their solution does not depend continuously on the data, and thus have to be solved via regularization techniques. Stable identification of space or/and time dependent parameters or source terms leads to (nonlinear) inverse problems typically governed by linear parabolic equations.

An important issue is also the availability of data: While for some applications, e.g., inverse problems in groundwater filtration, it is reasonable to assume distributed measurements (measurements of the state u on the whole domain), in many cases measurements will be possible only at the boundary. Thus, identification from a single set of or possibly multiple boundary measurements is of special interest.

In this section we consider a simple model problem (5.1) for a nonlinear diffusion process (we think of heat transfer and thus call u the 'temperature'), and show that, numerically, by either Newton method or Quasi-Newton method, a nonlinear source term $Q(u)$, can be uniquely and stably identified over a wide range of temperatures by the data of net flux γ_j on the boundary.

5.2 Newton method

In this section, we show how to reconstruct $Q(u)$ from finite data γ_j by a Newton scheme.

For any fixed $Q(u)$, the mapping from $Q(u)$ to the overposed data $\gamma_j(Q)$ is defined by

$$F : L^2 \rightarrow l_2, \quad F(Q) = \gamma_j(Q).$$

Theoretically, if we could show the invertibility of the Jacobian of the following mapping:

$$F(Q) = G_t(Q) - \gamma_j(Q),$$

where G_t is the corresponding value of γ_j after each iteration, and the map $G_t^N :$

$\mathbb{R}^N \mapsto \mathbb{R}^N$ is defined by

$$G_t^N = \begin{bmatrix} u_{1,x}(1, t; Q) - u_{1,x}(0, t; Q) \\ u_{2,x}(1, t; Q) - u_{2,x}(0, t; Q) \\ \vdots \\ u_{N,x}(1, t; Q) - u_{N,x}(0, t; Q) \end{bmatrix}$$

where $Q(u) = \sum_{i=1}^N q_i \psi_i(u)$ and $\mathbf{q} = (q_1, q_2, \dots, q_N)$, then the Newton scheme defined by

$$\mathbf{q}_{n+1} = \mathbf{q}_n - (\mathbf{D}G_t^N(\mathbf{q}_n))^{-1}[G_t^N(\mathbf{q}_n) - \gamma], \quad (5.2)$$

with γ being the net flux data, would be well-defined.

Even without any theoretical proofs we can attempt to use a Newton scheme which might give valuable insight to the problem and perhaps even give indications as to what restrictions might be necessary for a formal proof.

Example 5.2.1 Consider the inverse problem in the form

$$\begin{cases} \partial_t^\alpha u - u_{xx} = Q(u) + f_j(x, t), & 0 < x < 1, 0 < t < 1 \\ u_j(x, 0) = 0, & 0 < x < 1, \\ u_j(0, t) = u_j(1, t) = 0, & 0 \leq t \leq 1, \end{cases} \quad (5.3)$$

where the exact $Q(u) = -(u^2 + 3u)$, and we take

$$f_j(x, t) = \{1, \sin(2\pi x), \cos(2\pi x), \sin(4\pi x), \cos(4\pi x), \dots, \sin(8\pi x), \cos(8\pi x)\}.$$

We use polynomial basis set $\{1, u, u^2, \dots\}$ to express $Q(u)$ as

$$Q(u) = \sum_{n=0}^N q_n u^n,$$

and iterate the coefficients vector $\{q_n\}$. We stop the iteration if $\|q_{n+1} - q_n\|_{l^2} < \varepsilon$, where ε is the expected accuracy. With first guess $\{q_n\} = 0$, the graph of the exact Q and numerical Q is shown in Figure 5.1.

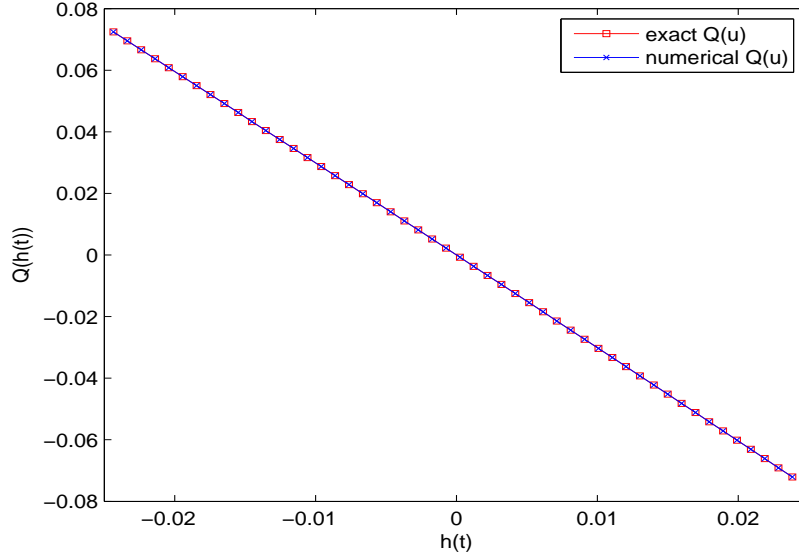


Figure 5.1: Example 5.2.1 Exact Q and numerical Q

5.3 Quasi-Newton method

In this section, we show how to numerically reconstruct $Q(u)$ from finite data γ_j by a Quasi-Newton scheme, with again the caveat that while each step follows a standard progression, we have no formal proofs for many of the steps.

We take $Q = 0$ in (5.2), namely we define the map $G_t^N : \mathbb{R}^N \mapsto \mathbb{R}^N$ by

$$G_t^N = \begin{bmatrix} u_{1,x}(1, t; 0) - u_{1,x}(0, t; 0) \\ u_{2,x}(1, t; 0) - u_{2,x}(0, t; 0) \\ \vdots \\ u_{N,x}(1, t; 0) - u_{N,x}(0, t; 0) \end{bmatrix}$$

where $Q(u)$ and \mathbf{q} are the same with before.

If we could show the invertibility of the Jacobian of mapping $F(Q)$, then the

Quasi-Newton scheme defined by

$$\mathbf{q}_{n+1} = \mathbf{q}_n - (\mathbf{D}G_t^N(\mathbf{q}_0))^{-1}[G_t^N(\mathbf{q}_n) - \gamma], \quad (5.4)$$

with γ being the net flux data, would be well-defined.

Example 5.3.1 Consider the inverse problem in the same form with Example 5.2.1 but the exact $Q(u) = -(u^2 + u)$, and we take

$$f_j(x, t) = \{1, \sin(2\pi x), \cos(2\pi x), \sin(4\pi x), \cos(4\pi x), \dots, \sin(8\pi x), \cos(8\pi x)\}.$$

We use polynomial basis set $\{1, u, u^2, \dots\}$ to express $Q(u)$ as

$$Q(u) = \sum_{n=0}^N q_n u^n.$$

We choose $Q_0 = 0$ and take first guess $\{q_n\} = 0$, then we iterate the vector of coefficients $\{q_n\}$ to get the proper approximation if we stop the iteration while $\|q_{n+1} - q_n\|_{l^2} < \varepsilon$, where ε is defined as above. The graph is shown in Figure 5.2.

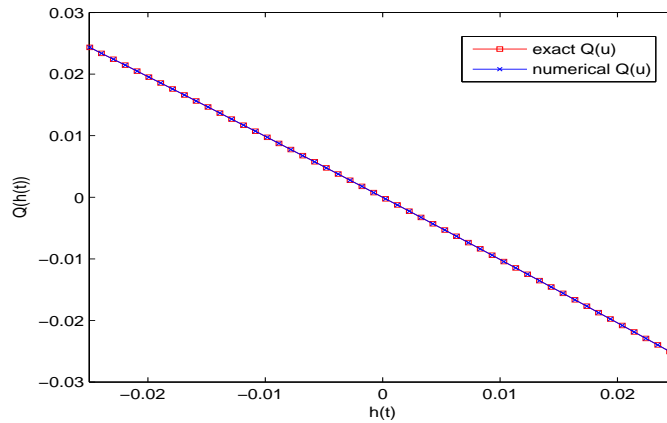


Figure 5.2: Example 5.3.1 Exact Q and numerical Q

6. CONCLUSION

Classical diffusion equations like the heat equation describe density or heat dynamics in a material undergoing diffusion. Its fundamental solution, a Gaussian distribution, has considerable useful properties and decays exponentially. The uniqueness and existence results of its solutions hold true under some assumptions of the initial conditions and boundary conditions. There exist maximum principles (weak and strong) that are useful for theoretical proof and numerical simulations.

Compared to the conventional diffusion described by the classical equation, *anomalous diffusion*, which shows radical differences, has been found and used recently. One anomalous diffusion corresponding to the time-fractional diffusion equation is called subdiffusion. It decays more slowly than the classical diffusion when time is large. Fractional diffusion equations still have existence and uniqueness results of the solutions under different assumptions on the initial and boundary conditions. But there are many more differences than similarities. There is no product rule or composite rule, so the integration by parts formula and many other useful tools for the classical differential equations also fail. This is a significant challenge for the analysis of fractional diffusion equations. The historical dependence property of the fractional derivative (either Riemann-Liouville type or Caputo type) requires more storage and computing time for numerical simulations.

Meanwhile, these different properties generate some new phenomena that are more advantageous than the classical one. The backward problem for fractional diffusion equations is only mildly ill-conditioned. The fractional Sturm-Liouville problem with the Caputo derivative only requires one Dirichlet spectrum to reconstruct the potential. This is the motivation for three inverse problems we have discussed

here.

Based on Mittag-Leffler functions and Wright functions, we constructed the fundamental solution for fractional diffusion equations and proved some properties to be used for the forward solutions. The forward solutions for fractional diffusion equations with either Dirichlet or Neumann boundary conditions were given explicitly by using the fundamental solutions we constructed. Some numerical schemes were discussed in order to solve inverse problems by the iteration method.

The first inverse problem we solved was the inverse boundary problem, where the nonlinear Neumann boundary condition is unknown but only related with the temperature. Given the overposed boundary data $u(0, t) = h(t)$, we applied the fixed point argument to recover this boundary condition. Uniqueness and existence results were discussed before we showed the validity of our method by two numerical examples. The role of the fractional derivative order was also probed by one numerical example.

If instead, the unknown nonlinear term is not on the boundary, but in the equation itself, for example, if a nonlinear term $f(u)$ on the right hand side of our fractional diffusion equation is unknown, could we still recover it by the same overposed data? The answer to this question was given in Section 4 where we still used the fixed point theory to show the uniqueness and existence result in the one-dimensional case. The uniqueness result was also given for a general space domain. One numerical example was listed to show the theory we proposed worked well.

Finally, we used different overposed data, the net flux, to reconstruct the same term as in Section 5. The problem was formulated and the Newton method and quasi-Newton method were applied to numerically reconstruct the unknown nonlinear term by multiple input sources. Two numerical examples were given to verify our scheme.

REFERENCES

- [1] Niels Abel: *Solution de quelques problemes a l'aide d'integrales definies*, *Oeuvres Completes*, Christiania (Grondahl), **1**(1881) pp.16-18.
- [2] E. E. Adams and L.W. Gelhar: *Field study of dispersion in heterogeneous aquifer 2. Spatial Moments Analysis*, *Water Resources Research*, **28** (1992) pp. 3293-3307.
- [3] R. A. Adams: *Sobolev Spaces*, Academic Press, New York, 1975.
- [4] O. M. Alifanov: *Inverse Heat Transfer Problems*, Springer, New York, 1994.
- [5] J. Beck, B. Blackwell, and C. S. Clair: *Inverse Heat Conductions*, Wiley, Sussex, 1985.
- [6] B. Berkowitz, A. Cortis, M. Dentz and H. Scher: *Modeling non-Fickian transport in geological formations as a continuous time random walk*, *Review of Geophysics*, **44** (2006) RG 2003/2006, Paper number 2005RG000178.
- [7] J. Cannon: *The One-Dimensional Heat Equation*, *Encyclopedia of Mathematics and its Applications*, 1984.
- [8] M. Caputo: *Elasticità e Dissipazione*, Zanichelli, Bologna, 1969.
- [9] A.S. Chaves: *A fractional diffusion equation to describe Levy flights*, *Physics Letters A*, **239** (1998) pp. 13-16.
- [10] J. Cheng, J. Nakagawa, M. Yamamoto and T. Yamazaki: *Uniqueness in an inverse problem for a one-dimensional fractional diffusion equation*, *Inverse Problems*, **25** (2009) 115002(16pp).

- [11] K. Diethelm: *The Analysis of Fractional Differential Equations. An Application-Oriented Exposition Using Operators of Caputo Type*, Lecture Notes in Mathematics, Springer-Verlag, Heidelberg, 2010.
- [12] K. Diethelm and N. J. Ford: *Multi-order fractional differential equations and their numerical solution*, Applied Mathematics and Computation, **154** (2004) pp. 621-640.
- [13] P. DuChateau and W. Rundell: *Unicity in an inverse problem for an unknown reaction term in a reaction diffusion equation*, Journal of Differential Equations, **59** (1985) pp. 155-164.
- [14] M.M. Dzhrbashyan: *Integral Transforms and Representations of Functions in Complex Domain*, Nauka, Moskow, 1966.
- [15] M.M. Dzhrbashyan and A.B. Nersesyan: *Fractional derivatives and the Cauchy problem for differential equations of fractional order*, Izvestiya Akademii Nauk SSSR. Seriya Matematicheskaya, **3**(1) (1968) pp. 3-29.
- [16] M.M. Dzhrbashyan, *A boundary value problem for a Sturm-Liouville type differential operator of fractional order*, Izvestiya Akademii Nauk SSSR. Seriya Matematicheskaya, **5**(2) (1970) pp.71-96.
- [17] M.M. Dzhrbashyan: *Harmonic Analysis and Boundary Value Problems in the Complex Domain*, Operator Theory: Advances and Applications, Birkhauser-Verlag, Berlin, 1993.
- [18] S.D. Eidelman and A.N. Kochubei: *Cauchy problem for fractional diffusion equations*, Journal of Differential Equations, **199** (2)(2004) pp. 211-255.

- [19] H. W. Engl and W. Rundell, editors: *Inverse Problems in Diffusion Processes*, SIAM, Philadelphia, 1994.
- [20] L.C. Evans, *Partial Differential Equations*, Graduate Studies in Mathematics, vol. 19, AMS, Providence, Rhode Island, 1998.
- [21] D. Gilbarg and N. S. Trudinger: *Elliptic Partial Differential Equations of Second Order*, Springer-Verlag, Berlin, 2001.
- [22] R. Gorenflo, Y. Luchko and F. Mainardi: *Analytical properties and applications of the Wright function*, Fractional Calculus and Applied Analysis, **2**(4) (1999) pp. 383-414.
- [23] W. Grever, A. Binder, H. W. Engl, and K. Mörwald: *Optimal cooling strategies in continuous casting of steel with variable casting speed*, Inverse Problems in Engineering, **2**(1997) pp.289-300.
- [24] G.B. Folland: *Real Analysis: Modern techniques and their applications*, John Wiley&Sons, Inc., New York, 1999
- [25] J. Fourier: *Analytical Theory of Heat*, *Analytical Theory of Heat*(*Great Books of the Western World, Vol. 45*), Encyclopedia Britannica, Inc., Chicago-London-Toronto, 1952.
- [26] A. Friedman: *Partial Differential Equations of Parabolic Type*, Robert E. Krieger, Inc., Malabar, Florida, 1983.
- [27] Y. Hatano and N. Hatano: *Dispersive transport of ions in column experiments: an explanation of long-tailed profiles*, Water Resources Research, **34** (1998) pp. 1027-1033.

- [28] B.T. Jin and W. Rundell: *An Inverse Sturm-Liouville Problem with a Fractional Derivative*, Journal of Computational Physics, **231**(2012) pp.4954-4966.
- [29] B.T. Jin and W. Rundell: *An inverse problem for a one-dimensional time-fractional diffusion problem*, Inverse Problems, **28**(2012) 075010(19 pp).
- [30] A.A. Kilbas, H.M Srivastava and J.J. Trujillo: *Theory and Applications of Fractional Differential Equations*, Elsevier, Amsterdam, 2006.
- [31] R. Kreß: *Linear Integral Equations*, Springer Verlag, Berlin, 1989.
- [32] S.F. Lacroix: *Traite du Calcul Differentiel et du Calcul Integral*, Second edition; Courcier, Paris, 1819.
- [33] Y. Lin and C. Xu: *Finite difference/spectral approximation for the time-fractional diffusion equation*, Journal of Computational Physics, **225** (2007) pp. 1533-1552.
- [34] V. Lipnevich and Y. Luchko: *The wright function: Its properties, applications, and numerical evaluation* , Applications of Mathematics in Technical and Natural Sciences, **1301**(2010) pp.614-622.
- [35] J.J. Liu and M. Yamamoto: *A backward problem for the time-fractional diffusion equation*, Applicable Analysis, **89** (2010) pp. 1769-1790.
- [36] Y. Luchko: *Maximum principle for the generalized time-fractional diffusion equation*, Journal of Mathematical Analysis and Applications, **351** (2009) pp. 218-223.
- [37] Yu. Luchko: *Algorithms for evaluation of the Wright function for the real arguments' values*, Fractional Calculus and Applied Analysis, **11**(2008) pp. 57-75.

- [38] F. Mainardi, Y. Luchko and G. Pagnini: *The fundamental solution of the space-time fractional diffusion equation*, Fractional Calculus and Applied Analysis, **4**(2) (2001) pp.153-192.
- [39] R. Metzler and J. Klafter: *The random walk's guide to anomalous diffusion: a fractional dynamics approach*, Physics Reports, **339** (2000) pp. 1-77.
- [40] K. S. Miller and B. Ross: *An Introduction to the Fractional Calculus and Fractional Differential Equations*, Wiley and Sons, New York, 1993.
- [41] G. M. Mittag-Leffler: *Sur la nouvelle fonction E_a* , Comptes Rendus de l'Académie des Sciences Paris, **137**(1903) pp. 554-558.
- [42] J. Nakagawa, K. Sakamoto and M. Yamamoto: *Overview to mathematical analysis for fractional diffusion equations-new mathematical aspects motivated by industrial collaboration*. Journal of Mathematics in Industry, **2A**(2010) pp. 99-108.
- [43] R.R. Nigmatullin: *The realization of the generalized transfer equation in a medium with fractal geometry*, Physica Status Solidi (b), **133**(1986) pp. 425-430.
- [44] K. B. Oldham and J. Spanier: *The Fractional Calculus*, Academic Press, New York, 1974.
- [45] M. Pilant and W. Rundell: *An iteration method for the determination of an unknown boundary condition in a parabolic initial boundary value problem*, Proceedings of the Edinburgh Mathematical Society, **32** (1989) pp. 59-71.

- [46] M. Pilant and W. Rundell: *An inverse problem for a nonlinear parabolic equation*, Communications in Partial Differential Equations, **11**(4) (1986) pp.445-457.
- [47] M. Pilant and W. Rundell *Undetermined coefficient problems for nonlinear elliptic and parabolic equations*, International Series of Numerical Mathematics, **77**(1986) pp.139-154.
- [48] M. Pilant and W. Rundell: *An inverse problem for a nonlinear elliptic equation*, SIAM Journal on Mathematical Analysis, **18**(6)(1987) pp.1801-1809.
- [49] M. Pilant and W. Rundell: *Iteration schemes for unknown coefficient problems arising in parabolic equations*, Numerical Methods for Partial Differential Equations, **3**(1987) pp.313-325.
- [50] I. Podlubny: *Fractional Differential Equations*, Academic Press, San Diego, 1999.
- [51] W.H. Press, B.P. Flannery, S.A. Teukolsky and W.T. Vetterling: *Numerical Recipes in C, The art of scientific Computing*, Cambridge University Press, Cambridge, 1988.
- [52] W. Rundell, X. Xu and L.H. Zuo: *The determination of an unknown boundary condition in a fractional diffusion equation*, Applicable Analysis (2012), DOI:10.1080/00036811.2012.686605.
- [53] K. Sakamoto and M. Yamamoto: *Initial value/boundary value problems for fractional diffusion-wave equations and applications to some inverse problems*, Journal of Mathematical Analysis and Applications, **382** (2011) pp.426-447.

- [54] I.M. Sokolov, J. Klafter and A. Blumen: *Fractional kinetics*, Physics Today, **55**(2002) pp.48-54.
- [55] A. B. Tayler: *Mathematical Models in Applied Mechanics*, Oxford University Press, 1986.
- [56] S.R. Umarov and E.M. Saidamatov: *A generalization of Duhamel's principle for differential equations of fractional order*, Doklady Mathematics, **75**(1) (2007) pp.94-96.
- [57] E.M. Wright: *On the coefficients of power series having exponential singularities*, Journal of the London Mathematical Society, **8**(1933) pp.71-79 .
- [58] E.M. Wright: *The asymptotic expansion of the generalized Bessel function*, Proceedings of the London Mathematical Society (Series II), **38** (1935) pp.257-270.
- [59] E.M. Wright: *The asymptotic expansion of the generalized hypergeometric function*, Journal of the London Mathematical Society, **10** (1935) pp.287-293 .
- [60] E.M. Wright: *The generalized Bessel function of order greater than one*, Quarterly Journal of Mathematics - Oxford, Oxford Series, **11** (1940) pp.36-48 .
- [61] L. Zhou and H.M. Selim: *Application of the fractional advection-dispersion equations in porous media*, Soil Science Society of America Journal, **67** (2003) pp.1079-1084.