Research Article

Xiangcheng Zheng, Yiqun Li, Jin Cheng and Hong Wang*

Inverting the variable fractional order in a variable-order space-fractional diffusion equation with variable diffusivity: Analysis and simulation

https://doi.org/10.1515/jiip-2019-0040
Received June 12, 2019; revised May 7, 2020; accepted September 27, 2020

Abstract: Variable-order space-fractional diffusion equations provide very competitive modeling capabilities of challenging phenomena, including anomalously superdiffusive transport of solutes in heterogeneous porous media, long-range spatial interactions and other applications, as well as eliminating the nonphysical boundary layers of the solutions to their constant-order analogues. In this paper, we prove the uniqueness of determining the variable fractional order of the homogeneous Dirichlet boundary-value problem of the one-sided linear variable-order space-fractional diffusion equation with some observed values of the unknown solutions near the boundary of the spatial domain. We base on the analysis to develop a spectral-Galerkin Levenberg–Marquardt method and a finite difference Levenberg–Marquardt method to numerically invert the variable order. We carry out numerical experiments to investigate the numerical performance of these methods.

Keywords: Inverse problem, variable-order space-fractional diffusion equation, uniqueness of the determination of the variable order, spectral-Galerkin method, finite difference method, Levenberg–Marquardt algorithm

MSC 2010: 35A20, 35R11, 35R30

1 Introduction

Fractional diffusion equations were derived under the assumptions that the probability density functions of the underlying particle movements exhibit highly skewed power-law decaying tails, so they can accurately describe the same behavior of the solute transport in heterogeneous media as observed in field experiments [3, 17, 21]. This explains why fractional diffusion equations model anomalously diffusive transport of solutes in heterogeneous aquifers more accurately than integer-order diffusion equations do [17–19]. However, the solutions to space-fractional diffusion equations exhibit singularities near the boundary, which is not common in the context of their integer-order counterparts [8].

Variable-order space-fractional diffusion equations, in which the fractional order varies in space, have shown to eliminate the nonphysical boundary layers that are present in the solutions to constant-order space-fractional diffusion equations and provide a physically relevant modeling [30]. Moreover, variable-order

***Corresponding author: Hong Wang,** Department of Mathematics, University of South Carolina, 1523 Greene Street, Columbia, South Carolina 29208, USA, e-mail: hwang@math.sc.edu
Xiangcheng Zheng, Yiqun Li, Department of Mathematics, University of South Carolina, 1523 Greene Street, Columbia, South Carolina 29208, USA, e-mail: xz3@math.sc.edu, yiqunl@email.sc.edu
Jin Cheng, School of Mathematical Sciences, Fudan University, 200433 Shanghai, P. R. China, e-mail: jcheng@fudan.edu.cn

space-fractional diffusion equations occur in many applications [16, 23, 24], as the order of space-fractional diffusion equations is closely related to the fractal dimension of the porous media determined by the Hurst index [7, 17] that change as the geometrical structure or property of the media changes.

In applications the parameters in the governing space-fractional diffusion equations, such as the variable fractional order, often are not given a priori. Rather, these parameters have to be inferred from the measurements as an inverse problem. In recent years, the inverse problems of determining the parameters in constant-order fractional diffusion equations, in particular the fractional order that was not encountered in the context of integer-order diffusion equations, have attracted extensive research activities [5, 9, 11–15, 29]. To our best knowledge, up to now, there is no mathematically proved result on the determination of the variable fractional order in variable-order space-fractional diffusion equations.

In this paper, we prove the uniqueness of the determination of the variable fractional order in the homogeneous Dirichlet boundary-value problem of one-sided linear variable-order space-fractional diffusion equations in one space dimension with measurements of the unknown solutions near the boundary of the spatial domain. Based on the analysis, we develop a spectral Galerkin Levenberg–Marquardt method and a finite difference Levenberg–Marquardt method to numerically invert the variable order. Numerical experiments are carried out to investigate the numerical performance of these methods.

The rest of the paper are organized as follows. In Section 2, we discuss the modeling issues and go over the wellposedness and regularity results of the problem. In Section 3, we prove that the variable fractional order of one-sided linear variable-order space-fractional diffusion equations can be uniquely determined, given the observations of the solutions near the boundary of the spatial domain. In Section 4, we develop a spectral Galerkin Levenberg–Marquardt method and a finite difference Levenberg–Marquardt method to numerically invert the variable fractional order. In Section 5, we carry out numerical experiments to investigate the performance of these methods. In Section 6, we draw concluding remarks.

2 A variable-order space-fractional diffusion equation model and its wellposedness

We address the modeling issues of space-fractional diffusion equations, and present a variable-order space-fractional diffusion equation model and go over its wellposedness and smoothing properties, which will be used subsequently.

2.1 Modeling issues by space-fractional diffusion equations

We begin with the homogeneous Dirichlet boundary-value problem of the one-sided space-fractional diffusion equation of order $1 < \alpha < 2$, which models the (one-sided) anomalously superdiffusive transport of the solutes in heterogeneous porous media [4, 10, 17, 25–28]

$$\begin{aligned} -{}_0^C D_x^\alpha u(x) &= f(x), \quad x \in [0,1], \\ u(0) &= u(1) = 0. \end{aligned} \tag{2.1}$$

Here the fractional integral operator ${}_0I_x^\beta$ of order $0 < \beta < 1$ and the Caputo fractional differential operator ${}_0^C D_x^\alpha$ of order $1 < \alpha < 2$ are defined by [20]

$$\begin{aligned} {}_0I_x^\beta g(x) &:= \frac{1}{\Gamma(\beta)} \int_0^x \frac{g(s)}{(x-s)^{1-\beta}}\, ds, \\ {}_0^C D_x^\alpha g(x) &:= {}_0I_x^{2-\alpha} g''(x) = \frac{1}{\Gamma(2-\alpha)} \int_0^x \frac{g''(s)}{(x-s)^{\alpha-1}}\, ds. \end{aligned} \tag{2.2}$$

We note that space-fractional diffusion equation (2.1) was derived via a continuous time random walk framework as the number of particle jumps tends to infinity (while the mean jump length shrinks) [17–19], and

hence holds for any fixed location x inside the domain that is away from the boundary and has nonlocal power law decaying tails, rather than all the way up to the boundary as often assumed in the literature [17–19]. This gap explains partially why the solutions to the boundary-value problem of space-fractional diffusion equation (2.1) exhibit nonphysical singularity near the left end point $x = 0$.

A time-dependent space-fractional diffusion equation model, which consists of a second-order spatial derivative term modeling the Fickian diffusive transport and a space-fractional derivative term modeling the superdiffusive transport, was proposed in [6, equation (29)] aiming at improving the modeling of superdiffusive transport. The steady-state counterpart of this model is presented as follows:

$$\begin{aligned} -u''(x) - k\,{}_0^C D_x^\alpha u(x) &= f(x), \quad x \in [0,1], \\ u(0) = u(1) &= 0, \end{aligned} \tag{2.3}$$

where u'' refers to the second-order derivative of u and ${}_0^C D_x^\alpha u$ was introduced in (2.1). Equation (2.3) can be well explained in the context of solute transport in heterogeneous porous media. During the transport process, a large amount of solute particles may transport through high permeability zones in a superdiffusive manner [3, 17] and may deviate from the transport of the solute particles in the bulk fluid phase that undergo a Fickian diffusive transport [2]. The partition parameter $k \geq 0$ quantifies the portion of the solute particles that move through the high permeability zones in a superdiffusive manner. That is, the $\frac{1}{1+k}$ portion of the total solute mass undergoes the Fickian diffusive transport, which is modeled by the $-u''$ term, while the remaining $\frac{k}{1+k}$ portion of the total solute mass undergoes the superdiffusive transport in high permeability zones and is modeled by $-k\,{}_0^C D_x^\alpha u$. Note that the governing space-fractional diffusion equation (2.3) holds on the entire spatial interval including the end point $x = 0$.

A possible remedy to eliminate the nonphysical singularity of the solutions to the boundary-value problem of space-fractional diffusion equation (2.1) (and (2.3)) as proved in [8] is to let the index of the power law decaying tails to very smoothly near the boundary of the domain to Gaussian types of tails to better reflect the impact of the boundary condition, or account for the impact of locality of the boundary condition at $x = 0$ from a mathematical point of view. This naturally leads to a (one-sided) variable-order space-fractional diffusion equation. Variable-order space-fractional diffusion equations occur in many applications, e.g., in modeling heterogeneous reservoirs that may consist of different types of heterogeneous porous media in different subdomains that naturally lead to different fractional orders in different subdomains.

Motivated by these observations, in this paper, we consider the homogeneous Dirichlet boundary-value problem of the (one-sided) variable-order linear space-fractional diffusion equation

$$\begin{aligned} -u''(x) - k(x)\,{}_0^C D_x^{\alpha(x)} u(x) &= f(x), \quad x \in (0,1), \\ u(0) = u(1) &= 0. \end{aligned} \tag{2.4}$$

Here ${}_0 I_x^{\beta(x)}$ with $0 < \beta(x) \leq 1$ and ${}_0^C D_x^{\alpha(x)}$ with $1 \leq \alpha(x) < 2$ denote the variable-order fractional integral and Caputo fractional differential operators, respectively [16, 23, 24]

$$\begin{aligned} {}_0 I_x^{\beta(x)} g(x) &:= \frac{1}{\Gamma(\beta(x))} \int_0^x \frac{g(s)}{(x-s)^{1-\beta(x)}}\, ds, \\ {}_0^C D_x^{\alpha(x)} g(x) &:= {}_0 I_x^{2-\alpha(x)} g''(x) = \frac{1}{\Gamma(2-\alpha(x))} \int_0^x \frac{g''(s)}{(x-s)^{\alpha(x)-1}}\, ds, \end{aligned}$$

which are variable-order extensions of the constant-order fractional integral and differential operators defined in (2.2).

2.2 Wellposedness and smoothing properties of variable-order space-fractional diffusion equation (2.4)

Let $C[0,1]$ be the Banach space of continuous functions defined on $[0,1]$, and let $C^m[0,1]$ be the Banach spaces of continuous functions with continuous derivatives up to order m on $[0,1]$, equipped with standard

norms [1]. We make the following assumptions on the variable order $\alpha(x)$, the partition coefficient $k(x)$ and the source term $f(x)$.

Assumption A. $\alpha, k, f \in C[0,1]$, $k \geq 0$, and α satisfies

$$\begin{gathered} 1 \leq \alpha(x) \leq \alpha_* := \max_{x\in[0,1]} \alpha(x) < 2, \quad x \in [0,1], \\ \lim_{x\to 0^+} (\alpha(x) - \alpha(0)) \ln x = 0. \end{gathered} \tag{2.5}$$

The following theorem was proved in [30].

Theorem 2.1. *Suppose that Assumption A holds. Then the homogeneous boundary-value problem* (2.4) *admits a unique solution* $u \in C^2[0,1]$. *Moreover, the following stability error estimate holds:*

$$\|u\|_{C^2[0,1]} \leq Q\|f\|_{C[0,1]},$$

where $Q = Q(\|k\|_{C[0,1]}, \|\alpha\|_{C[0,1]})$.

3 The unique determination of the variable order in problem (2.4)

In this section, we prove that the variable order $\alpha(x)$ in variable-order space-fractional diffusion equation (2.4) can be uniquely determined from the observations of the solution $u(x)$ on an arbitrarily small interval near the left end point of the interval. Let the admissible set $\mathcal{A}$ be defined by

$$\mathcal{A} := \{\alpha : \alpha \text{ is analytic on } [0,1] \text{ and satisfies (2.5)}\}.$$

We prove the main theoretical result of this paper in the following theorem.

Theorem 3.1. *Suppose that Assumption A holds and* $f(0), k(0) \neq 0$. *Then the variable order* $\alpha \in \mathcal{A}$ *in boundary-value problem* (2.4) *can be uniquely determined from the observations of the solution* $u(x)$ *on an arbitrarily small interval near the left end point of the interval. More precisely, let* $\hat{\alpha} \in \mathcal{A}$ *and* $\hat{u}(x)$ *be the solution to the problem*

$$\begin{gathered} -\hat{u}''(x) - k(x)\, {}_0^C D_x^{\hat{\alpha}(x)} \hat{u}(x) = f(x), \quad x \in (0,1), \\ \hat{u}(0) = \hat{u}(1) = 0. \end{gathered} \tag{3.1}$$

If there exists an ε_0 *with* $0 < \varepsilon_0 \ll 1$ *such that*

$$u(x) = \hat{u}(x) \quad \text{for all } x \in [0, \varepsilon_0], \tag{3.2}$$

then the following equation holds:

$$\alpha(x) = \hat{\alpha}(x) \quad \text{for all } x \in [0,1].$$

Proof. By Theorem 2.1, the solutions u to problem (2.4) and $\hat{u}$ to problem (3.1) satisfy $u, \hat{u} \in C^2[0,1]$. Thus, $v := u''$ and $\hat{v} := \hat{u}''$ satisfy the integral equations

$$\begin{aligned} v(x) + \frac{k(x)}{\Gamma(2-\alpha(x))} \int_0^x \frac{v(s)}{(x-s)^{\alpha(x)-1}}\, ds = -f(x) \quad \text{for all } x \in [0,1], \\ \hat{v}(x) + \frac{k(x)}{\Gamma(2-\hat{\alpha}(x))} \int_0^x \frac{\hat{v}(s)}{(x-s)^{\hat{\alpha}(x)-1}}\, ds = -f(x) \quad \text{for all } x \in [0,1]. \end{aligned} \tag{3.3}$$

By (3.2), $u(x) = \hat{u}(x)$ for all $x \in [0, \varepsilon_0]$. Thus, $v(x) = \hat{v}(x)$ for all $x \in [0, \varepsilon_0]$. Then we subtract the first equation in (3.3) from the second to deduce that

$$k(x) \int_0^x v(s) \Big(\frac{(x-s)^{1-\hat{\alpha}(x)}}{\Gamma(2-\hat{\alpha}(x))} - \frac{(x-s)^{1-\alpha(x)}}{\Gamma(2-\alpha(x))} \Big)\, ds = 0 \quad \text{for all } x \in [0, \varepsilon_0].$$

As $k(0) \neq 0$, there exists a constant $0 < \varepsilon_1 \leq \varepsilon_0$ such that $k(x) \neq 0$ for all $x \in [0, \varepsilon_1]$, which implies

$$\int_0^x v(s)\Big(\frac{(x-s)^{1-\hat{\alpha}(x)}}{\Gamma(2-\hat{\alpha}(x))} - \frac{(x-s)^{1-\alpha(x)}}{\Gamma(2-\alpha(x))}\Big)\,ds = 0, \quad x \in [0, \varepsilon_1]. \tag{3.4}$$

For any fixed $x \in (0, \varepsilon_1]$, $0 < s < x$ and $1 \leq \beta < 2$, let

$$G(\beta) := \frac{(x-s)^{1-\beta}}{\Gamma(2-\beta)}.$$

Then

$$\begin{aligned} G'(\beta) &= \Big(\frac{\Gamma'(2-\beta)}{\Gamma^2(2-\beta)}(x-s)^{1-\beta} - \frac{(x-s)^{1-\beta}\ln(x-s)}{\Gamma(2-\beta)}\Big) \\ &= \frac{(x-s)^{1-\beta}}{\Gamma(2-\beta)}\Big(\frac{\Gamma'(2-\beta)}{\Gamma(2-\beta)} - \ln(x-s)\Big) \quad \text{for all } 0 < s < x \text{ and all } x \in (0, \varepsilon_1]. \end{aligned} \tag{3.5}$$

Thus, (3.4) leads to

$$\begin{aligned} 0 &= \int_0^x v(s)\Big(\frac{(x-s)^{1-\hat{\alpha}(x)}}{\Gamma(2-\hat{\alpha}(x))} - \frac{(x-s)^{1-\alpha(x)}}{\Gamma(2-\alpha(x))}\Big)\,ds \\ &= \int_0^x v(s)[G(\hat{\alpha}(x)) - G(\alpha(x))]\,ds = \int_0^x v(s)G'(\bar{\alpha}(x))\,ds\,(\hat{\alpha}(x) - \alpha(x)), \end{aligned} \tag{3.6}$$

where $\bar{\alpha}(x)$ lies in between $\alpha(x)$ and $\hat{\alpha}(x)$ for any $x \in (0, \varepsilon_1]$.

We note that $v \in C[0, 1]$ and the kernel in the fractional integral of v in the first equation in (3.3) is weakly integrable. Hence, the fractional integral term in the equation vanishes as $x \to 0^+$. Moreover, by the assumptions of the theorem, $f \in C[0, 1]$ with $f(0) \neq 0$ which we assume to be positive without loss of generality. Hence, there exists a positive constant $0 < \varepsilon_2 \leq \varepsilon_1$ such that $f(x) > \frac{1}{2}f(0) > 0$ on $[0, \varepsilon_2]$. Then we conclude from the first equation in (3.3) that there exists a positive constant $0 < \varepsilon_3 \leq \varepsilon_2$ such that

$$v(x) \leq -\frac{f(0)}{4} < 0 \quad \text{for all } x \in [0, \varepsilon_3]. \tag{3.7}$$

By Assumption A,

$$2 - \alpha(x) \geq 2 - \alpha_* > 0, \quad 2 - \hat{\alpha}(x) \geq 2 - \alpha_* > 0.$$

Hence, $2 - \bar{\alpha}(x) \geq 2 - \alpha_* > 0$. There exist positive constants Q_1 and Q_2 such that

$$0 < Q_1 \leq \Gamma(x) \leq Q_2 < \infty, \quad 0 < Q_1 \leq |\Gamma'(x)| \leq Q_2 < \infty \quad \text{for all } x \in [2 - \alpha_*, 1].$$

Thus, there is a positive constant $Q_0 > 0$ such that

$$\Big|\frac{\Gamma'(2-\bar{\alpha}(x))}{\Gamma(2-\bar{\alpha}(x))}\Big| \leq Q_0, \quad x \in (0, \varepsilon_3].$$

Therefore, there exists a positive constant $0 < \varepsilon_4 \leq \varepsilon_3$ such that $\ln x < -2Q_0$ on $x \in (0, \varepsilon_4]$, which implies that

$$\frac{\Gamma'(2-\bar{\alpha}(x))}{\Gamma(2-\alpha(x))} - \ln(x-s) > Q_0 > 0 \quad \text{for all } 0 < s < x, \quad x \in (0, \varepsilon_4]. \tag{3.8}$$

We combine (3.5), (3.7) and (3.8) to conclude that

$$\begin{aligned} \int_0^x v(s)G'(\bar{\alpha}(x))\,ds &= \int_0^x v(s)\frac{(x-s)^{1-\bar{\alpha}(x)}}{\Gamma(2-\bar{\alpha}(x))}\Big(\frac{\Gamma'(2-\bar{\alpha}(x))}{\Gamma(2-\bar{\alpha}(x))} - \ln(x-s)\Big)\,ds \\ &< -\frac{Q_0 f(0)}{4}\int_0^x \frac{(x-s)^{1-\bar{\alpha}(x)}}{\Gamma(2-\bar{\alpha}(x))}\,ds = -\frac{Q_0 f(0)x^{2-\bar{\alpha}(x)}}{4\Gamma(3-\bar{\alpha}(x))} < 0 \quad \text{for all } x \in (0, \varepsilon_4]. \end{aligned} \tag{3.9}$$

We combine equations (3.6) and (3.9) to conclude that $\alpha(x) - \hat{\alpha}(x) = 0$ for $x \in (0, \varepsilon_4]$. As $\alpha(x)$ and $\hat{\alpha}(x)$ are analytical on [0,1], we deduce that $\alpha(x) \equiv \hat{\alpha}(x)$ for all $x \in [0, 1]$. □

4 Numerical inversion of the variable fractional order

We develop a spectral Galerkin Levenberg–Marquardt method and a finite difference Levenberg–Marquardt method to numerically invert the variable order $\alpha(x)$ in problem (2.4) from the observations of the solutions in a small interval near the left-end point.

4.1 A spectral Galerkin method to variable-order space-fractional diffusion equation (2.4)

Let $P_N[0, 1]$ be the space of polynomials of order less than or equal to N. For an integer $n \geq 0$, let $L_n(x)$ be the n-th Legendre polynomial on $[-1, 1]$ defined by the recurrence relation

$$\begin{aligned} L_0(x) &= 1, \quad L_1(x) = x, \\ L_{n+1}(x) &= \frac{2n+1}{n+1} x L_n(x) - \frac{n}{n+1} L_{n-1}(x), \quad n \geq 1 \end{aligned} \tag{4.1}$$

Let $\tilde{L}_n(x)$ be the shifted Legendre polynomial on the interval $[0, 1]$ by an affine mapping, and let

$$\phi_n(x) = \tilde{L}_n(x) - \tilde{L}_{n+2}(x), \quad n \geq 0.$$

Following [22, 28], we have $\phi_n(0) = \phi_n(1) = 0$ and

$$S_N[0, 1] := \{v \in P_N[0, 1] : v(0) = v(1) = 0\} = \operatorname{span}\{\phi_n\}_{n=0}^{N-2}.$$

Then the spectral Galerkin method for (2.4) reads: find $u_N \in S_N[0, 1]$ such that

$$(u_N', \phi_i') - (k\, {}_0^C D_x^\alpha u_N, \phi_i) = (f, \phi_i), \quad 0 \leq i \leq N-2. \tag{4.2}$$

4.2 A finite difference method to variable-order space-fractional diffusion equation (2.4)

Let $0 = x_0 < \cdots < x_K = 1$ be a uniform partition on $[0, 1]$ with the mesh size $h = \frac{1}{K}$. Then the two left-hand side terms of (2.4) can be discretized at $x = x_i$ (for $1 \leq i \leq K$) by

$$-u''(x_i) \approx -\frac{u(x_{i+1}) - 2u(x_i) + u(x_{i+1})}{h^2} =: -\delta_x^2 u(x_i)$$

and

$$\begin{aligned} -k(x_i)\, {}_0^C D_x^{\alpha(x)} u(x_i) &= \frac{-k(x_i)}{\Gamma(2-\alpha(x_i))} \int_0^{x_i} \frac{u''(s)}{(x-s)^{\alpha(x_i)-1}}\, ds \\ &\approx \frac{-k(x_i)}{\Gamma(2-\alpha(x_i))} \sum_{k=1}^{i} u''(x_k) \int_{x_{k-1}}^{x_k} \frac{1}{(x-s)^{\alpha(x_i)-1}}\, ds \\ &\approx \frac{-k(x_i)}{\Gamma(3-\alpha(x_i))} \sum_{k=1}^{i} \delta_x^2 u(x_k)\big((x_i - x_{k-1})^{2-\alpha(x_i)} - (x_i - x_k)^{2-\alpha(x_i)}\big) \\ &=: -k(x_i)\delta_x^\alpha u(x_i). \end{aligned}$$

Let u_i be an approximation to $u(x_i)$ for $1 \leq i \leq K-1$. We incorporate the preceding discretizations into space-fractional diffusion equation (2.4) to derive a finite difference method

$$-\delta_x^2 u_i - k(x_i)\delta_x^\alpha u_i = f(x_i), \quad 1 \leq i \leq K-1. \tag{4.3}$$

4.3 An inversion algorithm to evaluate the variable order $\alpha(x)$

With the spectral Galerkin method (4.2) and the finite difference method (4.3), we are now in the position to present an inversion algorithm to approximate the variable order $\alpha(x)$ that is formulated as follows.

Given the observation data $\{\theta_j\}_{j=1}^J$ measured at $\{\hat{x}_j\}_{j=1}^J$ in the interval $[0, \varepsilon_0]$ with $\varepsilon_0 < 1$, we aim at finding a numerical approximation $\alpha_M(x)$ to $\alpha(x)$, which is expressed in the form

$$\alpha_M(x) := \boldsymbol{\alpha}^\top \boldsymbol{\psi} \tag{4.4}$$

where

$$\boldsymbol{\alpha} := [\alpha_1, \ldots, \alpha_M]^\top, \quad \boldsymbol{\psi}(x) := [\psi_1(x), \ldots, \psi_M(x)]^\top$$

with $\{\psi_i\}_{i=1}^M$ being a set of basis functions. The goal is to minimize the discrete l_∞ error between the numerical solution of the spectral Galerkin method (4.2) or the finite difference method (4.3) to problem (2.4), with the variable-order $\alpha(x)$ being replaced by $\alpha_M(x)$ defined in (4.4), and the measurements $\{\theta_j\}_{j=1}^J$ at the measurement locations $\{\hat{x}_j\}_{j=1}^J$.

Let $u(x; \boldsymbol{\alpha})$ be the numerical solution of the spectral Galerkin method (4.2) or the finite difference method (4.3) to problem (2.4) with $\alpha(x)$ replaced by $\alpha_M(x)$ and $\boldsymbol{\alpha}$ introduced in (4.4), and let

$$\boldsymbol{u}(\boldsymbol{\alpha}) := [u(\hat{x}_1; \boldsymbol{\alpha}), u(\hat{x}_2; \boldsymbol{\alpha}), \ldots, u(\hat{x}_J; \boldsymbol{\alpha})]^\top.$$

The numerical approximation α_M is computed such that the corresponding coefficient $\boldsymbol{\alpha}$ minimizes the cost functional

$$\mathcal{F}(\boldsymbol{\alpha}) = \frac{1}{2} \sum_{j=1}^{J} (u(\hat{x}_j; \boldsymbol{\alpha}) - \theta_j)^2. \tag{4.5}$$

We use the Levenberg–Marquardt algorithm to iteratively minimize (4.5),

$$\boldsymbol{\alpha}_{k+1} := \boldsymbol{\alpha}_k - (\boldsymbol{J}_k^\top \boldsymbol{J}_k + \rho_k \boldsymbol{I})^{-1} \boldsymbol{J}_k^\top \boldsymbol{r}_k.$$

Here $\rho_k > 0$ is the regularization parameter, $\boldsymbol{r}_k := [u(\hat{x}_1; \boldsymbol{\alpha}_k) - \theta_1, \ldots, u(\hat{x}_J; \boldsymbol{\alpha}_k) - \theta_J]^\top$, and $\boldsymbol{J}_k$ is the Jacobian matrix of order $J \times M$,

$$\boldsymbol{J}_k := [\boldsymbol{j}_k^{\alpha_1}, \boldsymbol{j}_k^{\alpha_2}, \ldots, \boldsymbol{j}_k^{\alpha_M}],$$

which is evaluated via a numerical differentiation at $\boldsymbol{\alpha}_k$,

$$\boldsymbol{j}_k^{\alpha_j} = \frac{\boldsymbol{u}(\boldsymbol{\alpha}_k + \delta \boldsymbol{e}_j) - \boldsymbol{u}(\boldsymbol{\alpha}_k)}{\delta}, \quad j = 1, 2, \ldots, M, \tag{4.6}$$

where $\delta > 0$ is the numerical differentiation step size and $\boldsymbol{e}_j \in \mathbb{R}^J$ is the unit vector in the j-th coordinate direction for $j = 1, 2, \ldots, J$. The proposed parameter identification method is presented in Algorithm 1.

Algorithm 1. A Levenberg–Marquardt Algorithm

(i) Given the measurements $\boldsymbol{\theta}$ and the data for problem (2.4), choose the parameters $\rho \in (0, 1)$, $\sigma \in (0, 1)$, $\beta_0 > 0$, $0 < \delta \ll 1$, and an initial guess $\boldsymbol{\alpha}_0$. Set the iteration number $k := 0$.

(ii) Solve model (2.4) by (4.2) or (4.3) with α being replaced by α_M.

(iii) Use formula (4.6) to numerically compute Jacobian $\boldsymbol{J}_k$ and $\boldsymbol{J}_k^\top \boldsymbol{r}_k$.

(iv) Compute the search direction $\boldsymbol{d}_k := -(\boldsymbol{J}_k^\top \boldsymbol{J}_k)^{-1} \boldsymbol{J}_k^\top \boldsymbol{r}_k$.

(v) Determine the search step ρ^m by the Armijo rule: find the smallest possible m such that

$$\mathcal{F}(\boldsymbol{\alpha}_k + \rho^m \boldsymbol{d}_k) \le \mathcal{F}(\boldsymbol{\alpha}_k) + \sigma \rho^m \boldsymbol{d}_k \boldsymbol{J}_k^\top \mathbf{r}_k.$$

(vi) If $\|\rho^m \boldsymbol{d}_k\| < \text{tol}$, then stop, and let $\boldsymbol{\alpha} = \boldsymbol{\alpha}_k$. Otherwise, update $\boldsymbol{\alpha}_{k+1} := \boldsymbol{\alpha}_k + \rho^m \boldsymbol{d}_k$, $\beta_{k+1} := \frac{\beta_k}{2}$, $k := k + 1$, and turn to (ii).

5 Numerical experiments

We carry out numerical experiments to investigate the performance of the spectral Galerkin Levenberg–Marquardt method and the finite difference Levenberg–Marquardt method to invert the variable order $\alpha(x)$ in model (2.4), given the measurements on a sufficiently small interval $[0, \varepsilon_0]$ for some $\varepsilon_0 < 1$.

Example 1. Let $k(x) = 1$, $f(x) = 10$, $\alpha(x) = 1.5 + 0.1\sin(\pi x)$ in problem (2.4). In the Levenberg–Marquardt algorithm, we set $\rho = 0.75$, $\sigma = 0.25$, $\delta = 10^{-4}$ and tol $= 10^{-10}$. We choose $\{\psi_i(x)\}_{j=1}^{M}$ as the shifted Legendre polynomials (4.1) of orders up to $M-1$, $\varepsilon_0 = \frac{1}{8}$, $\frac{2}{8}$, $\frac{3}{8}$ and $\frac{4}{8}$ in (3.2), $M = 3$, 4, 5 and 6 in (4.4), and equally spaced observation points $\{\hat{x}_j\}_{j=1}^{J}$ with step size $d = \frac{1}{576}$. That is, $J = \frac{\varepsilon_0}{d}$, $\hat{x}_1 = d$ and $\hat{x}_J = \varepsilon_0$ on the interval $[0, \varepsilon_0]$. We choose $N = 10$ in the spectral Galerkin method (4.2) and $K = 576$ in the finite difference method (4.3) (so that the observation locations coincide with the mesh grids of the finite difference method on the interval $[0, \varepsilon_0]$). We choose the initial guess $\alpha \equiv 1.6$ in the Levenberg–Marquardt algorithm.

We present the error $\alpha - \alpha_M$ of the spectral Galerkin Levenberg–Marquardt algorithm, which is measured in the L_1, L_2 and L_∞ norms on $[0, 1]$, in Table 1 and the error $\alpha - \alpha_M$ of the finite difference Levenberg–Marquardt algorithm in Table 2, respectively. We present the plots of $\alpha(x)$ and $\alpha_M(x)$ as well as the values of the corresponding cost functionals, which are computed by the spectral Galerkin Levenberg–Marquardt algorithm and finite difference Levenberg–Marquardt algorithm with $M = 6$, in Figure 1.

We observe from Table 1 that the spectral Galerkin Levenberg–Marquardt method always generates a convergent numerical approximation α_M to α as M in (4.4) (and so the number of iterations) increases, which is independent of the size of the interval $[0, \varepsilon_0]$. As anticipated, if the size of the interval $[0, \varepsilon_0]$ of the measurements increases, the error $\alpha - \alpha_M$ is further improved. The finite difference Levenberg–Marquardt method is computationally more efficient than the spectral Galerkin Levenberg–Marquardt method. However, the numerical approximation α_M generated by the finite difference Levenberg–Marquardt method does not always converge monotonically as M increases.

These observations are consistent with the global nature of the spectral Galerkin method, which is computationally more expensive but tends to generate numerical approximations with better accuracy. On the other hand, the finite difference Levenberg–Marquardt method is computationally more efficient but may generate less accurate numerical approximations when the size of the observation interval is small, which is consistent with the local nature of the finite difference method.

$[J, \varepsilon_0]$	M	Itr	CPU time	$\|\alpha - \alpha_M\|_{L_\infty}$	$\|\alpha - \alpha_M\|_{L_2}$	$\|\alpha - \alpha_M\|_{L_1}$
$J = 72$, $\varepsilon_0 = \frac{1}{8}$	3	34	2m 55s	2.76E−01	1.17E−01	8.07E−02
	4	47	4m 50s	1.51E−01	4.45E−02	2.34E−02
	5	57	6m 50s	4.95E−02	1.44E−02	7.53E−03
	6	66	9m 8s	3.16E−02	8.39E−03	4.31E−03
$J = 144$, $\varepsilon_0 = \frac{2}{8}$	3	29	2m 30s	2.41E−01	1.01E−01	6.82E−02
	4	40	4m 7s	1.27E−01	3.67E−02	1.89E−02
	5	49	5m 55s	5.25E−02	1.53E−02	8.01E−03
	6	58	8m 0s	2.17E−02	6.85E−03	3.72E−03
$J = 216$, $\varepsilon_0 = \frac{3}{8}$	3	28	2m 26s	1.90E−01	7.80E−02	5.17E−02
	4	38	3m 55s	1.44E−01	5.61E−02	3.57E−02
	5	46	5m 34s	3.64E−02	1.15E−02	6.43E−03
	6	47	6m 33s	6.74E−03	2.61E−03	1.49E−03
$J = 288$, $\varepsilon_0 = \frac{4}{8}$	3	37	3m 12s	3.90E−02	1.72E−02	1.10E−02
	4	35	3m 38s	7.50E−02	3.00E−02	1.88E−02
	5	41	4m 56s	7.45E−03	2.36E−03	1.34E−03
	6	47	6m 34s	1.63E−03	7.14E−04	4.24E−04

Table 1: The error $\alpha - \alpha_M$ of the spectral Galerkin Levenberg–Marquardt algorithm with different values of ε_0 in Example 1

$[J, \varepsilon_0]$	M	Itr	CPU time	$\|\alpha - \alpha_M\|_{L_\infty}$	$\|\alpha - \alpha_M\|_{L_2}$	$\|\alpha - \alpha_M\|_{L_1}$
$J = 72, \varepsilon_0 = \frac{1}{8}$	3	40	22s	9.59E−02	3.90E−02	2.49E−02
	4	46	36s	1.33E−01	3.84E−02	1.98E−02
	5	58	1m 9s	6.30E−02	1.80E−02	9.17E−03
	6	54	1m 30s	1.14E−01	3.22E−02	1.68E−02
$J = 144, \varepsilon_0 = \frac{2}{8}$	3	35	16s	5.95E−02	2.47E−02	1.56E−02
	4	36	28s	1.17E−01	3.31E−02	1.67E−02
	5	48	57s	4.38E−02	1.24E−02	6.25E−03
	6	109	3m 2s	7.72E−02	2.11E−02	1.07E−02
$J = 216, \varepsilon_0 = \frac{3}{8}$	3	33	17s	3.36E−02	1.48E−02	9.42E−03
	4	35	30s	1.02E−01	2.84E−02	1.41E−02
	5	60	1m 18s	3.31E−02	9.33E−03	4.68E−03
	6	152	4m 24s	5.69E−03	2.00E−03	1.08E−03
$J = 288, \varepsilon_0 = \frac{4}{8}$	3	29	13s	3.83E−01	1.51E−01	9.93E−02
	4	32	26s	9.20E−02	2.54E−02	1.25E−02
	5	52	1m 3s	3.66E−02	1.03E−02	5.17E−03
	6	51	1m 26s	7.82E−03	2.52E−03	1.32E−03

Table 2: The error $\alpha - \alpha_M$ of the finite difference Levenberg–Marquardt algorithm with different values of ε_0 in Example 1

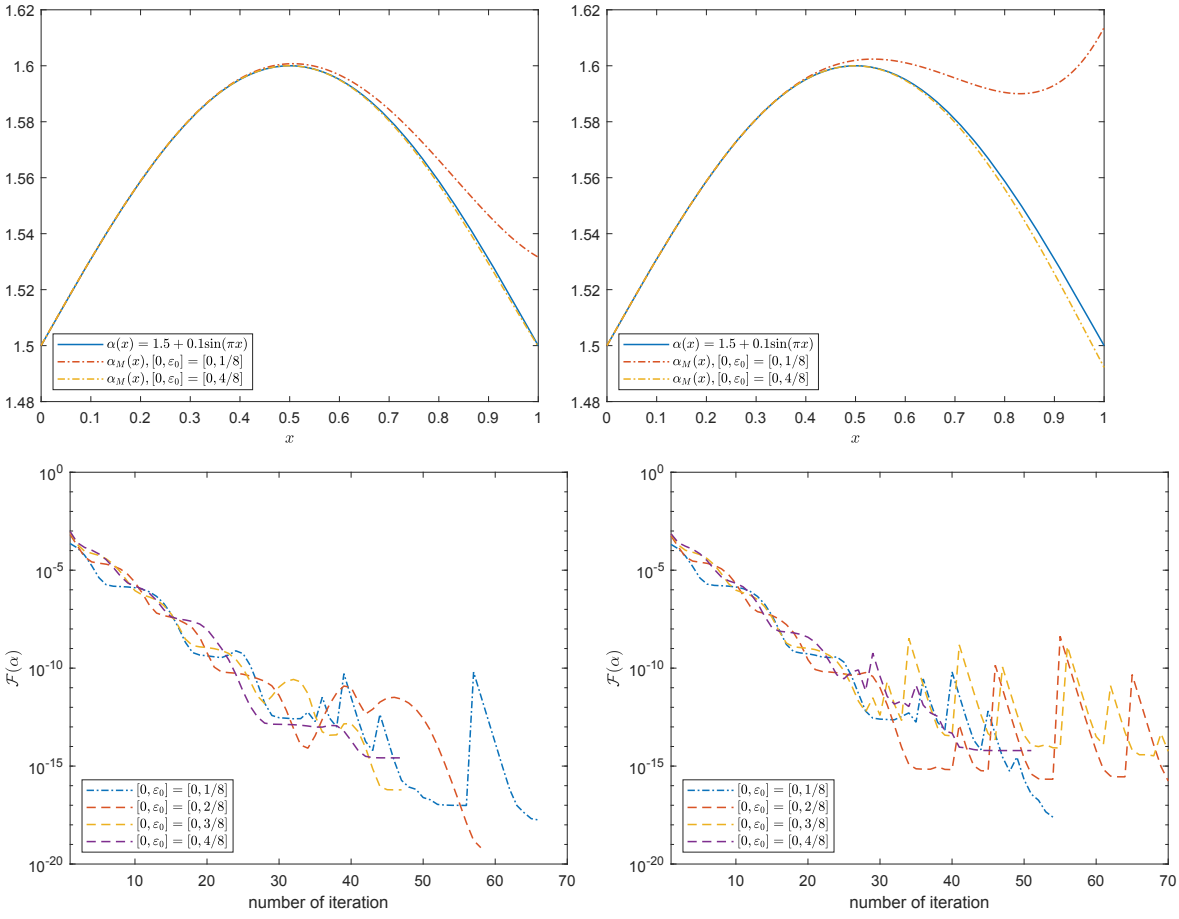

Figure 1: The plots of $\alpha(x)$ and $\alpha_M(x)$ (first row) and the values of the cost functional (second row), which are computed by the spectral Galerkin Levenberg–Marquardt algorithm (left) and the finite difference Levenberg–Marquardt algorithm (right) with different values of ε_0 in Example 1

$[J, \varepsilon_0]$	M	Itr	CPU time	$\|\alpha - \alpha_M\|_{L_\infty}$	$\|\alpha - \alpha_M\|_{L_2}$	$\|\alpha - \alpha_M\|_{L_1}$
$J = 72$, $\varepsilon_0 = \frac{1}{8}$	3	36	5m 9s	5.42E−02	1.59E−02	8.57E−03
	4	48	8m 15s	2.11E−02	5.80E−03	2.94E−03
	5	57	11m 41s	6.95E−03	1.80E−03	8.58E−04
	6	64	15m 3s	4.14E−03	9.73E−04	4.25E−04
$J = 144$, $\varepsilon_0 = \frac{2}{8}$	3	30	4m 18s	4.74E−02	1.35E−02	7.09E−03
	4	38	6m 32s	1.45E−02	3.80E−03	1.85E−03
	5	49	9m 50s	2.71E−03	6.62E−04	2.99E−04
	6	57	13m 18s	2.11E−03	4.78E−04	2.01E−04
$J = 216$, $\varepsilon_0 = \frac{3}{8}$	3	27	3m 58s	4.05E−02	1.12E−02	5.76E−03
	4	35	6m 12s	1.04E−02	2.62E−03	1.23E−03
	5	43	8m 52s	1.40E−03	3.25E−04	1.40E−04
	6	50	11m 34s	8.26E−04	1.78E−04	7.13E−05
$J = 288$, $\varepsilon_0 = \frac{4}{8}$	3	21	3m 3s	3.39E−02	9.01E−03	4.66E−03
	4	34	5m 53s	7.35E−03	1.78E−03	8.09E−04
	5	41	8m 16s	8.05E−04	1.78E−04	7.34E−05
	6	47	6m 47s	3.36E−04	6.84E−05	2.59E−05

Table 3: The error $\alpha - \alpha_M$ of the spectral Galerkin Levenberg–Marquardt algorithm with different values of ε_0 in Example 2

$[J, \varepsilon_0]$	M	Itr	CPU time	$\|\alpha - \alpha_M\|_{L_\infty}$	$\|\alpha - \alpha_M\|_{L_2}$	$\|\alpha - \alpha_M\|_{L_1}$
$J = 72$, $\varepsilon_0 = \frac{1}{8}$	3	36	17s	5.42E−02	1.59E−02	8.57E−03
	4	65	50s	2.08E−02	5.70E−03	2.88E−03
	5	62	1m 14s	1.12E−02	2.93E−03	1.42E−03
	6	58	1m 37s	2.40E−02	6.24E−03	3.01E−03
$J = 144$, $\varepsilon_0 = \frac{2}{8}$	3	30	14s	4.74E−02	1.35E−02	7.09E−03
	4	44	34s	1.46E−02	3.83E−03	1.86E−03
	5	55	1m 5s	2.52E−03	6.13E−04	2.76E−04
	6	63	1m 46s	9.80E−04	2.10E−04	8.38E−05
$J = 216$, $\varepsilon_0 = \frac{3}{8}$	3	27	12s	4.05E−02	1.12E−02	5.76E−03
	4	35	27s	1.04E−02	2.63E−03	1.23E−03
	5	48	57s	1.45E−03	3.36E−04	1.45E−04
	6	48	1m 21s	1.18E−03	2.57E−04	1.04E−04
$J = 288$, $\varepsilon_0 = \frac{4}{8}$	3	21	10s	3.39E−02	9.01E−03	4.66E−03
	4	34	28s	7.34E−03	1.77E−03	8.07E−04
	5	43	52s	8.09E−04	1.79E−04	7.38E−05
	6	47	1m 20s	3.67E−04	7.51E−05	2.86E−05

Table 4: The error $\alpha - \alpha_M$ of the finite difference Levenberg–Marquardt algorithm with different values of ε_0 in Example 2

Example 2. We choose $\alpha(x) = 0.1x^{11/3} + 1.1$ in problem (2.4) and the initial guess $\alpha \equiv 1.3$ in the Levenberg–Marquardt algorithm. All the other data are chosen the same as those in Example 1. We present the results in Tables 3 and 4, respectively, and in Figure 2. We reach the same observations as those in Example 1.

6 Concluding remarks

In this paper, we proved the unique determination of the variable fractional order of the homogeneous Dirichlet boundary-value problem of the one-sided linear variable-order space-fractional diffusion equation with some observed values of the unknown solutions near the boundary of the spatial domain. We accordingly developed a spectral Galerkin Levenberg–Marquardt algorithm and a finite difference Levenberg–Marquardt algorithm to numerically invert the variable order. We carried out numerical experiments to

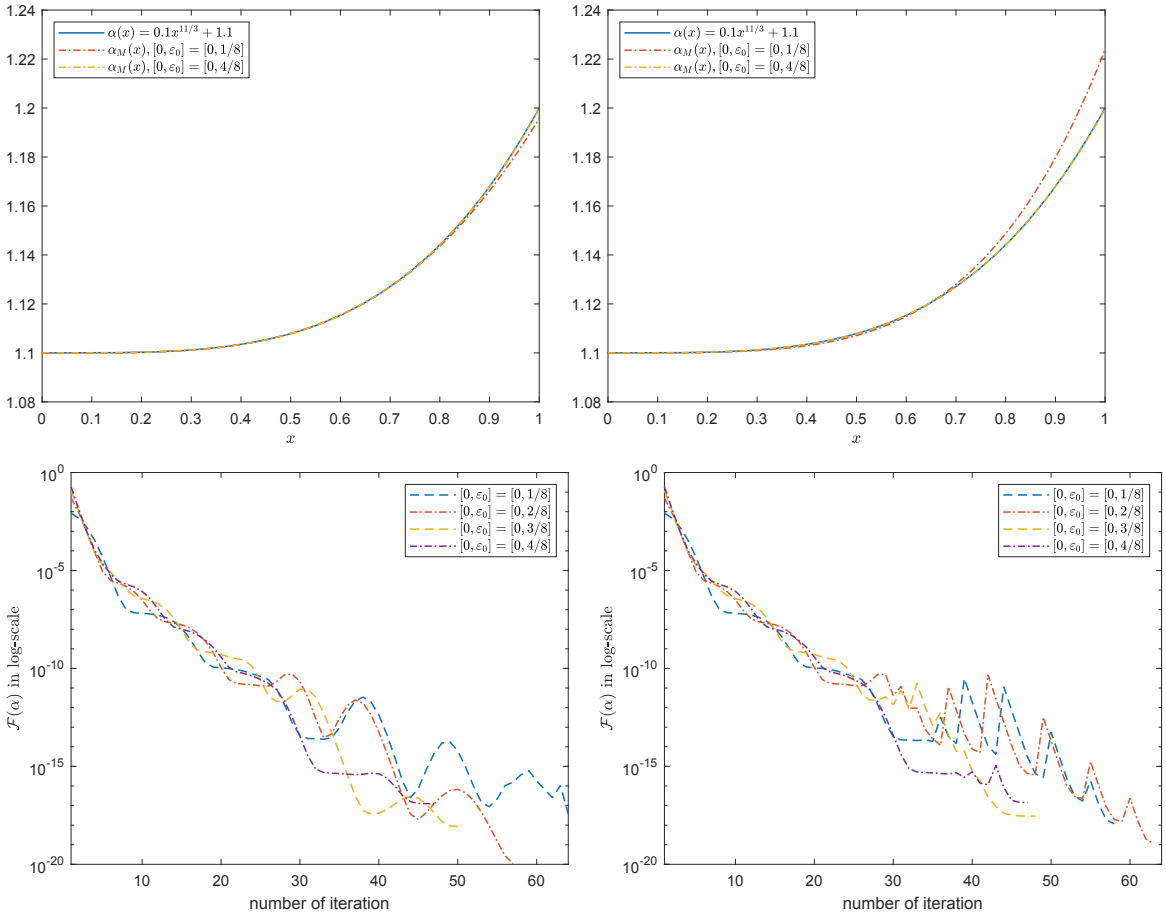

Figure 2: The plots of $\alpha(x)$ and $\alpha_M(x)$ (first row) and the values of the cost functional (second row), which are computed by the spectral Galerkin Levenberg–Marquardt algorithm (left) and the finite difference Levenberg–Marquardt algorithm (right) with different values of ε_0 in Example 2

investigate the convergence behavior of the numerical approximations to the variable order generated by both methods, from the observed data only on a small interval near the boundary.

We conclude this paper by commenting on the analytical assumption of the variable order $\alpha(x)$ in problem (2.4). The analysis technique in this paper was developed to conclude that the positive- (or negative-) preserving property of the integral on the left-hand side of (3.9) on a sufficiently small interval, which in turn leads to $\alpha(x) = \hat{\alpha}(x)$ on this interval. Then the analytic assumption on α was used to show that all the derivatives of α at $x = 0$ are uniquely determined, which in turn uniquely determines $\alpha(x)$ on the entire interval $[0, 1]$ since α is analytic.

Conceptually, unless the fractional order is constant, it is intuitively impossible to use the value of the variable order $\alpha(x)$ on a sufficiently small interval $[0, \varepsilon_0]$ to uniquely determine the value of $\alpha(x)$ on the entire interval $[0, 1]$ for a general variable order $\alpha(x)$ that is not analytical. It seems that any reasonable relaxation of the analytical assumption on the variable order $\alpha(x)$ should require more observations of the unknown solution u on the interval $[0, 1]$. While requiring the observation of the solution $u(x)$ on the entire interval $[0, 1]$ probably does not make much sense, the authors are currently looking for appropriately specified observations of the solution $u(x)$ to problem (2.4) on the interval $[0, 1]$ such that the unique identification of the variable order $\alpha(x)$ in problem (2.4) can be proved without the analytical assumption on $\alpha(x)$.

Acknowledgment: The authors would like to express their most sincere thanks to the referees for their helpful comments and suggestions, which greatly improved the quality of this paper.

Funding: This work was partially funded by the ARO MURI Grant W911NF-15-1-0562, by the National Science Foundation under Grants DMS-1620194 and DMS-2012291, by the National Natural Science Foundation of China under Grants 11421110002 and 11971272, and by a SPARC Graduate Research Grant from the Office of the Vice President for Research at the University of South Carolina.

References

[1] R. A. Adams and J. J. F. Fournier, *Sobolev Spaces*, Elsevier, San Diego, 2003.
[2] J. Bear, *Dynamics of Fluids in Porous Media*, Elsevier, New York, 1972.
[3] D. A. Benson, R. Schumer, M. M. Meerschaert and S. W. Wheatcraft, Fractional dispersion, Lévy motion, and the MADE tracer tests, *Transp. Porous Media* **42** (2001), no. 1–2, 211–240.
[4] P. Carr and L. R. Wu, The finite moment logstable process and option pricing, *J. Finance* **58** (2003), 753–778.
[5] 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), no. 11, Article ID 115002.
[6] D. del Castillo-Negrete, Front propagation in reaction-diffusion systems with anomalous diffusion, *Bol. Soc. Mat. Mex. (3)* **20** (2014), no. 1, 87–105.
[7] P. Embrechts and M. Maejima, *Selfsimilar Processes*, Princeton Ser. Appl. Math., Princeton University, Princeton, 2002.
[8] V. J. Ervin, N. Heuer and J. P. Roop, Regularity of the solution to 1-D fractional order diffusion equations, *Math. Comp.* **87** (2018), no. 313, 2273–2294.
[9] J. Janno, Determination of the order of fractional derivative and a kernel in an inverse problem for a generalized time fractional diffusion equation, *Electron. J. Differential Equations* **2016** (2016), Paper No. 199, 28.
[10] B. Jin, R. Lazarov, J. Pasciak and W. Rundell, Variational formulation of problems involving fractional order differential operators, *Math. Comp.* **84** (2015), no. 296, 2665–2700.
[11] B. Jin and W. Rundell, An inverse problem for a one-dimensional time-fractional diffusion problem, *Inverse Problems* **28** (2012), no. 7, Article ID 075010.
[12] Y. Kian, L. Oksanen, E. Soccorsi and M. Yamamoto, Global uniqueness in an inverse problem for time fractional diffusion equations, *J. Differential Equations* **264** (2018), no. 2, 1146–1170.
[13] G. Li, D. Zhang, X. Jia and M. Yamamoto, Simultaneous inversion for the space-dependent diffusion coefficient and the fractional order in the time-fractional diffusion equation, *Inverse Problems* **29** (2013), no. 6, Article ID 065014.
[14] Z. Li, Y. Liu and M. Yamamoto, Inverse problems of determining parameters of the fractional partial differential equations, in: *Handbook of Fractional Calculus with Applications. Vol. 2*, De Gruyter, Berlin (2019), 431–442.
[15] J. J. Liu and M. Yamamoto, A backward problem for the time-fractional diffusion equation, *Appl. Anal.* **89** (2010), no. 11, 1769–1788.
[16] C. F. Lorenzo and T. T. Hartley, Variable order and distributed order fractional operators, *Nonlinear Dyn.* **29** (2002), no. 1–4, 57–98.
[17] M. M. Meerschaert and A. Sikorskii, *Stochastic Models for Fractional Calculus*, De Gruyter Stud. Math. 43, Walter de Gruyter, Berlin, 2012.
[18] R. Metzler and J. Klafter, The random walk's guide to anomalous diffusion: A fractional dynamics approach, *Phys. Rep.* **339** (2000), no. 1, 1–77.
[19] R. Metzler and J. Klafter, The restaurant at the end of the random walk: Recent developments in the description of anomalous transport by fractional dynamics, *J. Phys. A* **37** (2004), no. 31, R161–R208.
[20] S. G. Samko, A. A. Kilbas and O. I. Marichev, *Fractional Integrals and Derivatives: Theory and Applications*, Gordon and Breach Science, Yverdon, 1993.
[21] R. Schumer, D. A. Benson, M. M. Meerschaert and S. W. Wheatcraft, Eulerian derivation of the fractional advection-dispersion equation, *J. Contaminant Hydrol.* **48** (2001), 69–88.
[22] J. Shen, T. Tang and L.-L. Wang, *Spectral Methods*, Springer Ser. Comput. Math. 41, Springer, Heidelberg, 2011.
[23] H. Sun, A. Chang, Y. Zhang and W. Chen, A review on variable-order fractional differential equations: Mathematical foundations, physical models, numerical methods and applications, *Fract. Calc. Appl. Anal.* **22** (2019), no. 1, 27–59.
[24] H. Sun, W. Chen and Y. Chen, Variable-order fractional differential operators in anomalous diffusion modeling, *Phys. A* **388** (2009), 4586–4592.
[25] H. Wang and D. Yang, Wellposedness of variable-coefficient conservative fractional elliptic differential equations, *SIAM J. Numer. Anal.* **51** (2013), no. 2, 1088–1107.
[26] H. Wang, D. Yang and S. Zhu, Inhomogeneous Dirichlet boundary-value problems of space-fractional diffusion equations and their finite element approximations, *SIAM J. Numer. Anal.* **52** (2014), no. 3, 1292–1310.
[27] H. Wang, D. Yang and S. Zhu, Accuracy of finite element methods for boundary-value problems of steady-state fractional diffusion equations, *J. Sci. Comput.* **70** (2017), no. 1, 429–449.

[28] H. Wang and X. Zhang, A high-accuracy preserving spectral Galerkin method for the Dirichlet boundary-value problem of variable-coefficient conservative fractional diffusion equations, *J. Comput. Phys.* **281** (2015), 67–81.
[29] X. Xu, J. Cheng and M. Yamamoto, Carleman estimate for a fractional diffusion equation with half order and application, *Appl. Anal.* **90** (2011), no. 9, 1355–1371.
[30] X. Zheng and H. Wang, An optimal-order numerical approximation to variable-order space-fractional diffusion equations on uniform or graded meshes, *SIAM J. Numer. Anal.* **58** (2020), no. 1, 330–352.