

A finite difference method for space fractional differential equations with variable diffusivity coefficient ^{*}

K. Mustapha, K. Furati, O. M. Knio, O. P. Le Maître

June 3, 2017

Abstract

Anomalous diffusion is a phenomenon that cannot be modeled accurately by second-order diffusion equations, but is better described by fractional diffusion models. The nonlocal nature of the fractional diffusion operators makes substantially more difficult the mathematical analysis of these models and the establishment of suitable numerical schemes. This paper proposes and analyzes the first finite difference method for solving *variable-coefficient* fractional differential equations, with two-sided fractional derivatives, in one-dimensional space. The proposed scheme combines first-order forward and backward Euler methods for approximating the left-sided fractional derivative when the right-sided fractional derivative is approximated by two consecutive applications of the first-order backward Euler method. Our finite difference scheme reduces to the standard second-order central difference scheme in the absence of fractional derivatives. The existence and uniqueness of the solution for the proposed scheme are proved, and truncation errors of order h are demonstrated, where h denotes the maximum space step size. The numerical tests illustrate the global $O(h)$ accuracy of our scheme, except for nonsmooth cases which, as expected, have deteriorated convergence rates.

1 Introduction

This work aims at constructing and analyzing a finite difference scheme for solving one-dimensional two-sided conservative fractional order differential equations with variable coefficient, κ , of the form:

$$-\partial_x (\kappa(x) \partial_x^{\alpha, \theta} u(x)) = f(x), \quad \text{for } x \in \Omega := (a, b), \quad (1)$$

where $\alpha \in (0, 1)$ is the fractional order exponent and κ is the generalized diffusivity coefficient satisfying the positivity assumption $c_0 \leq \kappa(x) \leq c_1$ on Ω , for some positive constants c_0 and c_1 . In (1), ∂_x denotes the first-order derivative and $\partial_x^{\alpha, \theta}$ the two-sided fractional order differential operator defined by

$$\partial_x^{\alpha, \theta} \phi := \theta {}_a D_x^\alpha \phi + (1 - \theta) {}_x D_b^\alpha \phi.$$

Here, $0 \leq \theta \leq 1$ is a parameter describing the relative probabilities of particles to travel ahead or behind the mean displacement, ${}_a D_x^\alpha$ and ${}_x D_b^\alpha$ are left-sided (LS) and right-sided (RS) Riemann-Liouville fractional derivatives (with respect to x), defined respectively as

$${}_a D_x^\alpha v(x) := \frac{\partial}{\partial x} {}_a I_x^{1-\alpha} v(x) = \frac{\partial}{\partial x} \int_a^x \omega_{1-\alpha}(x-z) v(z) dz,$$

and

$${}_x D_b^\alpha v(x) := \frac{\partial}{\partial x} {}_x I_b^{1-\alpha} v(x) = \frac{\partial}{\partial x} \int_x^b \omega_{1-\alpha}(z-x) v(z) dz.$$

^{*}The support of the KFUPM through the project No. KAUST005 is gratefully acknowledged

[†]Research reported in this publication was supported by research funding from King Abdullah University of Science and Technology (KAUST).

In the previous expressions, we denoted ${}_a I_x^{1-\alpha}$ and ${}_x I_b^{1-\alpha}$ the LS and RS Riemann-Liouville fractional integrals, respectively, with kernel $\omega_{1-\alpha}(x) := \frac{x^{-\alpha}}{\Gamma(1-\alpha)}$, where Γ is the classical gamma function.

We shall consider boundary conditions of Dirichlet type for the solution of (1), that is,

$$u(a) = d_1 \quad \text{and} \quad u(b) = d_2. \quad (2)$$

Without loss of generality, we assume in the following that $d_1 = d_2 = 0$, that is, homogeneous Dirichlet boundary conditions. If $d_1 \neq 0$ or $d_2 \neq 0$, we substitute

$$u(x) = w(x) + \tilde{u}(x), \quad \tilde{u}(x) := \frac{x-a}{b-a}d_2 + \frac{b-x}{b-a}d_1,$$

in (1), and solve for w subject to homogeneous Dirichlet boundary conditions, $w(a) = w(b) = 0$, and modified source term function $\tilde{f} := f + \partial_x(\kappa \partial_x^{\alpha, \theta} \tilde{u})$. The practical evaluation of \tilde{f} can follow the approach outlined in A.

In the limiting case $\alpha = 1$, the fractional derivative ∂_x^α reduces to ∂_x and the problem (1)–(2) reduces to the classical two-point elliptic boundary value problem, where $-\kappa \partial_x u$ is the ordinary diffusion flux from the Fick's law, Fourier's law, or Newtonian constitutive equation. An implied assumption is that the rate of diffusion at a certain location is independent of the global structure of the diffusing field. In the last few decades, an increasing number diffusion processes were found to be non-Fickian, and anomalous diffusion has been experimentally documented in many applications of interest [2, 19, 22] (*e.g.*, viscoelastic materials, subsurface flows and plasma physics). In these situations, the mean square displacement grows in time faster (superdiffusion) or slower (subdiffusion) than that in a normal (Gaussian) diffusion process. This deviation from normal diffusion can be explained by non-Newtonian mechanics and Lévy processes. In such phenomena, the anomalous diffusion rate is affected not only by the local conditions (gradient) but also by the global state of the field. For instance, the time fractional derivative acting on the diffusion term (subdiffusion) [19] accommodates the existence of long-range correlations in the particle dynamics. Similarly, space fractional derivatives, which are suitable for the modeling of superdiffusion processes, account for anomalously large particle jumps at a rate inconsistent with the classical Brownian motion model. At the macroscopic level, these jumps give rise to a spatial fractional diffusion equation [2, 4]:

$$\partial_t u - \partial_x(\kappa \partial_x^{\alpha, \theta} u) = g. \quad (3)$$

In most studies, the diffusion coefficient κ is assumed to be constant, and the process to be symmetric [2, 7]. In this case, $\theta = 1/2$, (1) reduces to the Riesz fractional derivative of order $1 + \alpha$, and many numerical methods have been proposed for its solution, see [3, 8, 10, 13, 14, 15, 16, 21, 24, 26, 27, 31, 32] and related references therein. However, many practical problems require a model with variable diffusion coefficients κ [1, 5], and the asymmetric diffusion process seems inherent in some physical systems [6, 23].

The model problem (1) is the steady state form of model problem (3). For a constant diffusivity κ , the operator $\partial_x(\kappa \partial_x^{\alpha, \theta})$ is a linear combination of the LS and RS fractional derivatives of order $\alpha + 1$. Let $\langle \cdot, \cdot \rangle$ be the classical L_2 -inner product over Ω and $H_0^\mu(\Omega)$, with $\mu < 1/2$, the fractional Sobolev space of order μ of functions with zero trace on $\partial\Omega$. For the Galerkin weak formulation of (1), we seek the solution $u \in H_0^{1-\beta}(\Omega)$, with $\beta = (1 - \alpha)/2$, such that

$$\mathcal{A}(u, v) = \langle f, v \rangle, \quad \forall v \in H_0^{1-\beta}(\Omega), \quad (4)$$

where the bilinear form $\mathcal{A} : H_0^{1-\beta/2}(\Omega) \times H_0^{1-\beta/2}(\Omega) \rightarrow \mathbb{R}$, is defined by

$$\mathcal{A}(v, w) := -\kappa[\theta \langle {}_a D_x^{1-\beta} v, {}_x D_1^{1-\beta} w \rangle + (1 - \theta) \langle {}_x D_1^{1-\beta} v, {}_a D_x^{1-\beta} w \rangle].$$

Ervin and Roop [11] investigated the well-posedness of the Galerkin formulation (4) for constant κ . They proved that the bilinear form \mathcal{A} is then coercive and continuous on $H_0^{1-\beta/2}(\Omega) \times H_0^{1-\beta/2}(\Omega) \rightarrow \mathbb{R}$, and hence, that (4) has a unique solution $u \in H_0^{1-\beta}(\Omega)$ in this case. For a rigorous study of the variational formulation of (1) when κ is constant and $\theta = 1$, we refer to [12].

Unfortunately, it was shown in [28] that the Galerkin formulation loses coercivity on $H_0^{1-\beta/2}(\Omega) \times H_0^{1-\beta/2}(\Omega) \rightarrow \mathbb{R}$ in the variable-coefficient case and the authors even propose a counterexample in the

symmetric case ($\theta = 1$, see [28, Lemma 3.2]). As a result, the weak formulation (4) is not an appropriate framework for variable coefficient κ , as the Galerkin finite element methods might fail to converge [29]. As an alternative, a Petrov-Galerkin method was investigated in [30] for the case of LS fractional derivatives ($\theta = 1$). For the same setting, a finite difference method was proposed and analyzed in [25].

It is worth to mention that extending existing numerical methods from constant to variable diffusivity is not straightforward, if feasible at all, because of the presence fractional order derivatives. Similarly, the analyses of the generic problem (1) remain scarce due to the mathematical difficulties induced by LS and RL nonlocal operators, that prevent reusing the results of classical elliptic equations. Therefore, the main motivation of the present work is to approximate the solution of (1) *via* finite difference methods, for variable diffusivity κ and allowing skewness parameter $0 \leq \theta \leq 1$. Specifically, we consider numerical schemes based on appropriate combinations of first-order backward and forward differences. For convenience, we first develop and analyze in Section 2 a finite difference scheme for (1) with $\theta = 1$, that is, we have to deal with the LS fractional derivative only. Then, in Section 3, the other limiting case $\theta = 0$ with RS fractional derivative only is considered. The contributions of both LS and RL fractional derivatives are subsequently combined in Section 4, to derive the generic finite difference scheme for (1) that reduces to the classical second-order central difference scheme in the limiting case $\alpha = 1$. For each case, we prove the existence and uniqueness of the finite difference solution and show $O(h)$ truncation errors for the resulting schemes, (h is the maximum space step size). We present several numerical experiments in Section 5 to support our theoretical convergence results in the case of smooth and non-smooth solutions. Finally, Section 6 provides concluding remarks and recommendations for future works.

2 LS fractional derivative

We start by introducing several notations and definitions. For the discretization of the problem, we consider a partition of Ω with P subintervals $I_{1 \leq n \leq P}$ constructed using a sequence of $(P + 1)$ points such that $a = x_0 < x_1 < x_2 < \dots < x_P = b$. Unless stated otherwise, we shall restrict ourselves to the case of uniform partitions with spatial step size $h = x_n - x_{n-1} = (b - a)/P$. We shall denote $x_{n+1/2} = (x_n + x_{n+1})/2$ the center of interval I_{n+1} . Denoting $v^n := v(x_n)$, we use the symbol δv^n to denote the backward difference defined as

$$\delta v(x) = \delta v^n := v^n - v^{n-1}, \quad \forall x \in I_n.$$

2.1 Finite difference scheme

Equation (1) with $\theta = 1$ reduces to

$$-\partial_x (\kappa(x) {}_a D_x^\alpha u)(x) = f(x). \quad (5)$$

Using first a forward type difference treatment of the operator ∂_x , we propose the following approximation

$$\partial_x (\kappa {}_a D_x^\alpha u)(x_n) \approx h^{-1} \left[\kappa^{n+1/2} {}_a D_x^\alpha u(x_{n+1}) - \kappa^{n-1/2} {}_a D_x^\alpha u(x_n) \right], \quad (6)$$

where $\kappa^{n+1/2} := \kappa(x_{n+1/2})$. Observe that the proposed scheme involves a half-cell shift in the localization of the values of κ (at the cells centers), for reasons that will become clear from the analysis below.

Remarking that ${}_a D_x^\alpha u = {}_a I_x^{1-\alpha} u'$, because $u(0) = 0$, equation (6) can be recast as

$$\partial_x (\kappa {}_a D_x^\alpha u)(x_n) \approx h^{-1} [\kappa^{n+1/2} {}_a I_x^{1-\alpha} u'(x_{n+1}) - \kappa^{n-1/2} {}_a I_x^{1-\alpha} u'(x_n)].$$

Applying now the backward difference approximation to the derivatives inside the integrals, results in

$$\partial_x (\kappa {}_a D_x^\alpha u)(x_n) \approx h^{-2} [\kappa^{n+1/2} ({}_a I_x^{1-\alpha} \delta u)(x_{n+1}) - \kappa^{n-1/2} ({}_a I_x^{1-\alpha} \delta u)(x_n)],$$

for $n = 1, \dots, P-1$. In addition, we have

$$\begin{aligned} {}_a I_x^{1-\alpha} \delta u(x_n) &= \sum_{j=1}^n \int_{I_j} \omega_{1-\alpha}(x_n - s) \delta u^j ds = \omega_{2-\alpha}(h) \sum_{j=1}^n w_{n,j} \delta u^j \\ &= \omega_{2-\alpha}(h) \left(\sum_{j=1}^{n-1} [w_{n,j} - w_{n,j+1}] u^j + u^n \right), \end{aligned} \quad (7)$$

with the weights defined as

$$w_{n,j} := (n+1-j)^{1-\alpha} - (n-j)^{1-\alpha} \quad \text{for } n \geq j \geq 1. \quad (8)$$

We denote by $U^n \approx u^n$ the finite difference solution, which for the model problem in (5) is required to satisfy

$$\kappa^{n-1/2} ({}_a I_x^{1-\alpha} \delta U)(x_n) - \kappa^{n+1/2} ({}_a I_x^{1-\alpha} \delta U)(x_{n+1}) = h^2 f^n, \quad (9)$$

for $n = 1, \dots, P-1$, with $U^0 = U^P = 0$. Using (7), the finite difference scheme can be recast as

$$\kappa^{n-1/2} \sum_{j=1}^n w_{n,j} \delta U^j - \kappa^{n+1/2} \sum_{j=1}^{n+1} w_{n+1,j} \delta U^j = \tilde{f}_h^n, \quad (10)$$

with the modified right-hand-side

$$\tilde{f}_h^n := \frac{h^2}{\omega_{2-\alpha}(h)} f^n. \quad (11)$$

For computational convenience, the finite difference scheme (9) can be expressed as

$$\begin{aligned} \sum_{j=1}^{n-1} \left(\kappa^{n-1/2} [w_{n,j} - w_{n,j+1}] - \kappa^{n+1/2} [w_{n+1,j} - w_{n+1,j+1}] \right) U^j \\ + \left(\kappa^{n-1/2} - \kappa^{n+1/2} (2^{1-\alpha} - 2) \right) U^n - \kappa^{n+1/2} U^{n+1} = \tilde{f}_h^n, \end{aligned}$$

or in the compact form:

$$\sum_{j=1}^n \left(a_{n,j} - a_{n+1,j} \right) U^j - \kappa^{n+1/2} U^{n+1} = \tilde{f}_h^n, \quad \text{for } n = 1, \dots, P-1,$$

where

$$a_{n,j \leq n} = \begin{cases} \kappa^{n-1/2} & j = n, \\ \kappa^{n-1/2} [w_{n,j} - w_{n-1,j}] & j < n. \end{cases}$$

The finite difference solution is then obtained solving the $(P-1)$ -by- $(P-1)$ linear system $\mathbf{B}_L \mathbf{U} = \mathbf{F}$, where $\mathbf{U} = [U^1, U^2, \dots, U^{P-1}]^T$, $\mathbf{F} = [\tilde{f}_h^1, \tilde{f}_h^2, \dots, \tilde{f}_h^{P-1}]^T$, and

$$\mathbf{B}_L = \begin{bmatrix} c_{1,1} & -\kappa^{3/2} & 0 & \cdots & \cdots & 0 \\ c_{2,1} & c_{2,2} & -\kappa^{5/2} & 0 & \cdots & \vdots \\ c_{3,1} & c_{3,2} & c_{3,3} & -\kappa^{7/2} & \ddots & \vdots \\ \vdots & \vdots & & \ddots & \ddots & \\ \vdots & \vdots & & & & 0 \\ c_{P-2,1} & c_{P-2,2} & \cdots & \cdots & c_{P-2,P-2} & -\kappa^{P-3/2} \\ c_{P-1,1} & c_{P-1,2} & \cdots & \cdots & c_{P-1,P-2} & c_{P-1,P-1} \end{bmatrix}, \quad (12)$$

with

$$c_{n,j} = \begin{cases} \kappa^{n-1/2} - \kappa^{n+1/2} [2^{1-\alpha} - 2] & j = n, \\ a_{n,j} - a_{n+1,j} & j < n. \end{cases}$$

Remark 1. For the case of a constant diffusivity, say $\kappa = 1$, the matrix \mathbf{B}_L reduces to the Toeplitz form,

$$\mathbf{B}_L = \begin{bmatrix} d_1 & -1 & 0 & \cdots & \cdots & 0 \\ d_2 & d_1 & -1 & 0 & \cdots & \vdots \\ d_3 & d_2 & d_1 & -1 & \ddots & \vdots \\ \vdots & \vdots & & \ddots & \ddots & \\ \vdots & \vdots & & & & 0 \\ d_{P-2} & d_{P-3} & \cdots & \cdots & d_1 & -1 \\ d_{P-1} & d_{P-2} & \cdots & \cdots & d_2 & d_1 \end{bmatrix},$$

where $d_1 = 3 - 2^{1-\alpha} > 1$ and $d_j = -(j+1)^{1-\alpha} + 3j^{1-\alpha} - 3(j-1)^{1-\alpha} + (j-2)^{1-\alpha}$, for $2 \leq j \leq P-1$.

Remark 2. As mentioned earlier, in the limiting case $\alpha = 1$, equation (1) reduces to the classical elliptic problem $-\partial_x(\kappa\partial_x u) = f$. Furthermore, the finite difference scheme (9) reduces to

$$\kappa^{n+1/2}\delta U^{n+1} - \kappa^{n-1/2}\delta U^n = h^2 f^n,$$

for $n = 1, \dots, P-1$. This is the classical second order difference scheme for the elliptic problems. In this case, one can easily check that the system matrix \mathbf{B}_L becomes tridiagonal and symmetric, with entries $c_{i,j} = 0$ for $|i-j| > 2$, $c_{i,i+1} = -\kappa^{i+1/2}$, $c_{i,i} = \kappa^{i-1/2} + \kappa^{i+1/2}$ and $c_{i,i-1} = -\kappa^{i-1/2}$.

2.2 Existence and uniqueness

This subsection is devoted to study the existence and uniqueness of the finite difference solution U^n . Because it satisfies the a square linear system of equations, the existence of the finite difference solution follows from its uniqueness. To prove uniqueness, we need to show that the finite difference solution is identically zero when $f = 0$, that is when the system right-hand-side is zero, that is $f^j = 0$ for $j = 1, \dots, P-1$. To do so, we multiply both sides of (10) by U^n and sum over index n ; using $U^P = 0$ we have

$$\sum_{n=1}^P U^n \kappa^{n-1/2} \sum_{j=1}^n w_{n,j} \delta U^j - \sum_{n=1}^{P-1} U^n \kappa^{n+1/2} \sum_{j=1}^{n+1} w_{n+1,j} \delta U^j = 0. \quad (13)$$

Because $U^0 = 0$, the second term on the left-hand side gives

$$\sum_{n=2}^P U^{n-1} \kappa^{n-1/2} \sum_{j=1}^n w_{n,j} \delta U^j = \sum_{n=1}^P U^{n-1} \kappa^{n-1/2} \sum_{j=1}^n w_{n,j} \delta U^j,$$

and substituting back in (13) we obtain

$$\sum_{n=1}^P \kappa^{n-1/2} \delta U^n \left(\sum_{j=1}^n w_{n,j} \delta U^j \right) = 0.$$

This equality can be expressed in a matrix form,

$$\Phi \mathbf{A} \mathbf{W}_\alpha \Phi^T = \mathbf{0}, \quad (14)$$

where $\Phi = [\delta U^1, \delta U^2, \dots, \delta U^P]$ with its transpose Φ^T . In equation (14), the matrix \mathbf{W}_α is P -by- P lower triangular, with entries $w_{n,j}$ for $1 \leq j \leq n \leq P$, while \mathbf{A} is diagonal with entries $\mathbf{A}_{n,n} = \kappa^{n-1/2}$. One can easily check that all eigenvalues of $\mathbf{A} \mathbf{W}_\alpha$ are positive. Thus, $\mathbf{A} \mathbf{W}_\alpha$ is positive definite matrix, and equation (14) implies $\Phi \equiv \mathbf{0}$. Consequently, the finite difference solution U^n is identically zero, for $1 \leq n \leq P-1$, because $U^0 = U^P = 0$. This completes the proof of the existence and uniqueness of the finite difference solution U .

2.3 Truncation error

We now turn to establishing the truncation error of the proposed scheme. From (5) and (9), the truncation error T_h^n is given by

$$T_h^n = \partial_x(\kappa_a D_x^\alpha u)(x_n) - \frac{1}{h^2} \left(\kappa^{n+1/2} ({}_a I_x^{1-\alpha} \delta u)(x_{n+1}) - \kappa^{n-1/2} ({}_a I_x^{1-\alpha} \delta u)(x_n) \right).$$

Since

$$\begin{aligned} h \partial_x(\kappa_a D_x^\alpha u)(x_n) &= \int_{I_{n+1}} f(x_n) dx = \int_{I_{n+1}} [f(x_n) - f(x)] dx + \int_{I_{n+1}} \partial_x(\kappa_a D_x^\alpha u)(x) dx \\ &= - \int_{I_{n+1}} \int_{x_n}^x f'(t) dt dx + \kappa^{n+1} {}_a I_x^{1-\alpha} u'(x_{n+1}) - \kappa^n {}_a I_x^{1-\alpha} u'(x_n), \end{aligned}$$

we have

$$T_h^n = -\frac{1}{h} \int_{I_{n+1}} \int_{x_n}^x f'(t) dt dx + G_h^n - Q_h^n,$$

where

$$G_h^n = \frac{1}{h} \left[\kappa^{n+1} {}_a I_x^{1-\alpha} u'(x_{n+1}) - \kappa^n {}_a I_x^{1-\alpha} u'(x_n) \right], \quad Q_h^n = \frac{1}{h^2} \left[\kappa^{n+1/2} {}_a I_x^{1-\alpha} \delta u(x_{n+1}) - \kappa^{n-1/2} {}_a I_x^{1-\alpha} \delta u(x_n) \right].$$

Using the change of variable $s = q + h$, we observe that

$$\begin{aligned} {}_a I_x^{1-\alpha} u'(x_{n+1}) &= \sum_{j=1}^{n+1} \int_{I_j} \omega_{1-\alpha}(x_{n+1} - s) u'(s) ds \\ &= \int_{I_1} \omega_{1-\alpha}(x_{n+1} - s) u'(s) ds + \sum_{j=1}^n \int_{I_j} \omega_{1-\alpha}(x_n - q) u'(q + h) dq. \end{aligned}$$

Similarly, for the backward difference we have

$$\begin{aligned} {}_a I_x^{1-\alpha} \delta u(x_{n+1}) &= \sum_{j=1}^{n+1} \int_{I_j} \omega_{1-\alpha}(x_{n+1} - s) \delta u^j ds \\ &= \delta u^1 \int_{I_1} \omega_{1-\alpha}(x_{n+1} - s) ds + \sum_{j=1}^n \delta u^{j+1} \int_{I_j} \omega_{1-\alpha}(x_n - q) dq. \end{aligned}$$

Therefore, the truncation error can be rewritten as

$$T_h^n = -\frac{1}{h} \int_{I_{n+1}} \int_{x_n}^x f'(t) dt + E_1^n + \sum_{j=1}^n \int_{I_j} \omega_{1-\alpha}(x_n - q) E_2^{n,j}(q) dq, \quad \text{for } n \geq 1,$$

where

$$E_1^n := \int_{I_1} \omega_{1-\alpha}(x_{n+1} - s) [h^{-1} \kappa^{n+1} u'(s) - h^{-2} \kappa^{n+1/2} u^1] ds,$$

and

$$E_2^{n,j}(q) := \frac{\kappa^{n+1} u'(q + h) - \kappa^n u'(q)}{h} - \frac{\kappa^{n+1/2} \delta u^{j+1} - \kappa^{n-1/2} \delta u^j}{h^2}.$$

Focusing on the second error contribution, E_1^n , we observe that for sufficient smoothness, specifically for $\kappa \in C^1(I_{n+1})$ and $u \in C^2(a, x_1]$, we have for $s \in I_1$ (at leading order)

$$\kappa^{n+1/2} u^1 = [\kappa^{n+1} + O(h)] [h u'(x_1) + O(h^2)] = h \kappa^{n+1} u'(s) + O(h^2).$$

Consequently, an application of the mean value theorem for integral yields

$$E_1^n = O(1) \int_{I_1} \omega_{1-\alpha}(x_{n+1} - s) ds = O(h)(x_{n+1} - \xi)^{-\alpha}, \quad \text{for some } \xi \in I_1. \quad (15)$$

Regarding the last error contribution in T_h^n above, we first remark that for any $q \in (x_{j-1}, x_j)$, one has

$$\kappa^{n+1}u'(q+h) - \kappa^n u'(q) = \kappa^n[u'(q+h) - u'(q)] + [\kappa^{n+1} - \kappa^n]u'(q+h),$$

and that, for $\kappa \in C^2[x_{n-1}, x_{n+1}]$ and $u \in C^3[x_{j-1}, x_{j+1}]$, Taylor series expansions give

$$\begin{aligned} \kappa^{n+1/2}\delta u^{j+1} - \kappa^{n-1/2}\delta u^j &= [(\kappa^{n+1/2} - \kappa^n) + \kappa^n][\delta u^{j+1} - \delta u^j] + [\kappa^{n+1/2} - \kappa^{n-1/2}]\delta u^j \\ &= h^2\left[\frac{h}{2}\kappa'(x_n) + \kappa^n\right]u''(x_j) + h^2\kappa'(x_n)u'(x_j) + O(h^3), \end{aligned}$$

Gathering the previous results, we obtain for $E_2^{n,j}$

$$\begin{aligned} E_2^{n,j}(q) &= h^{-1}\kappa^n[u'(q+h) - u'(q) - hu''(x_j)] \\ &\quad + h^{-1}[\kappa^{n+1} - \kappa^n - h\kappa'(x^n)]u'(q+h) + \kappa'(x^n)[u'(q+h) - u'(x_j)] \\ &= -h^{-1}\kappa^n \int_q^{q+h} \int_t^{x_j} u'''(x) dx dt + \frac{h}{2}\kappa''(\xi^n)u'(q+h) + \kappa'(x^n) \int_{x_j}^{q+h} u''(x) dx, \end{aligned}$$

for some $\xi^n \in I_{n+1}$. This shows that the first double integral term is $O(h^2)$ when $u \in C^3[x_{j-1}, x_{j+1}]$, whereas the second term is $O(h)$ for $\kappa \in C^2(\bar{I}_{n+1})$ and $u \in C^1(\bar{I}_{j+1})$ and the third one is $O(h)$ for $\kappa \in C^1(\bar{I}_{n+1})$ and $u \in C^2(\bar{I}_{j+1})$. This results leads to the conclusion that the last error contribution to T_h^n is $O(h)$. Putting all these estimates together, we obtain that for $f \in C^1(\bar{\Omega})$, $\kappa \in C^2(\bar{\Omega})$ and $u \in C^3(\bar{\Omega})$ the truncation error is

$$T_h^n = O(h)(1 + (x_n - a)^{-\alpha}), \quad \text{for } 1 \leq n \leq P-1.$$

Therefore, for $0 < \alpha < 1$, the truncation error T_h^n is of order h for x_n not too close to the left boundary $x = a$.

3 RS fractional derivative

In this section, we focus on the finite difference approximation of problem (1) when $\theta = 0$, that is, the RS fractional elliptic problem:

$$-\partial_x(\kappa_x D_b^\alpha u)(x) = f(x). \quad (16)$$

We shall rely on the same notations as in the previous section.

3.1 Finite difference scheme

Contrary to the case of the LS fractional derivative, we propose a backward difference type treatment for the differential operator ∂_x , and consider the approximation

$$\partial_x(\kappa_x D_b^\alpha u)(x_n) \approx h^{-1}[\kappa^{n+1/2} {}_x D_b^\alpha u(x_n) - \kappa^{n-1/2} {}_x D_b^\alpha u(x_{n-1})].$$

Again, observe the shift in the evaluation points for κ (at the cell centers) compared to fractional differential operator (at the mesh point), which is crucial to ensure the recovery of the classical second order scheme when $\alpha \rightarrow 1$. Noting that ${}_x D_b^\alpha u = {}_x I_b^{1-\alpha} u'$, because $u(1) = 0$, we have

$$\partial_x(\kappa_x D_b^\alpha u)(x_n) \approx h^{-1} \left[\kappa^{n+1/2} {}_x I_b^{1-\alpha} u'(x_n) - \kappa^{n-1/2} {}_x I_b^{1-\alpha} u'(x_{n-1}) \right].$$

Applying the backward difference to the derivatives inside the integrals, one gets

$$\partial_x(\kappa_x D_b^\alpha u)(x_n) \approx h^{-2} \left[\kappa^{n+1/2} ({}_x I_b^{1-\alpha} \delta u)(x_n) - \kappa^{n-1/2} ({}_x I_b^{1-\alpha} \delta u)(x_{n-1}) \right], \quad \text{for } n = 1, \dots, P-1.$$

The finite difference solution $U^n \approx u^n$ of the (RS) fractional model problem (16) satisfies the system:

$$\kappa^{n-1/2}({}_x I_b^{1-\alpha} \delta U)(x_{n-1}) - \kappa^{n+1/2}({}_x I_b^{1-\alpha} \delta U)(x_n) = h^2 f^n, \quad (17)$$

for $n = 1, \dots, P-1$, complemented by the boundary conditions $U^0 = U^P = 0$.

Further, application of the integral form of the RS Riemann-Liouville fractional derivative to the finite difference, δv , yields:

$${}_x I_b^{1-\alpha} \delta v(x_{n-1}) = \sum_{j=n}^P \int_{I_j} \omega_{1-\alpha}(s - x_{n-1}) \delta v^j ds = \omega_{2-\alpha}(h) \sum_{j=n}^P w_{j,n} \delta v^j,$$

such that the numerical scheme (17) can be expressed as

$$\kappa^{n-1/2} \sum_{j=n}^P w_{j,n} \delta U^j - \kappa^{n+1/2} \sum_{j=n+1}^P w_{j,n+1} \delta U^j = \tilde{f}_h^n. \quad (18)$$

In equation (17), the weights $w_{n,j}$ and modified right-hand side \tilde{f}_h^n follow the definitions of the previous section, see equations (8) and (11) respectively. Making use of the equality

$$\sum_{j=n}^P w_{j,n} \delta v^j = \sum_{j=n}^{P-1} [w_{j,n} - w_{j+1,n}] v^j - w_{n,n} v^{n-1},$$

the finite difference scheme (17) can be rewritten as

$$\sum_{j=n}^{P-1} (b_{jn} - b_{j,n+1}) U^j - \kappa^{n-1/2} U^{n-1} = \tilde{f}_h^n, \quad n = 1, \dots, P-1,$$

where $b_{n,n+1} = -\kappa^{n+1/2}$ and $b_{j,n} = \kappa^{n-1/2} [w_{j,n} - w_{j,n-1}]$ for $j \geq n$.

The finite difference solution of the RS fractional diffusion problem is thus obtained by solving the $(P-1)$ -by- $(P-1)$ linear system $\mathbf{B}_R \mathbf{U} = \mathbf{F}$, with the system matrix

$$\mathbf{B}_R = \begin{bmatrix} d_{1,1} & d_{1,2} & d_{1,3} & d_{1,4} & d_{1,5} & \cdots & d_{1,P-1} \\ -\kappa^{3/2} & d_{2,2} & d_{2,3} & d_{2,4} & d_{2,5} & \cdots & d_{2,P-1} \\ 0 & -\kappa^{5/2} & d_{3,3} & b_{3,4} & d_{3,5} & \cdots & d_{3,P-1} \\ 0 & 0 & -\kappa^{7/2} & d_{4,4} & b_{4,5} & \cdots & d_{4,P-1} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \cdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & -\kappa^{P-3/2} & d_{P-1,P-1} \end{bmatrix}$$

having upper-triagonal entries

$$d_{n,j} = \begin{cases} -\kappa^{n-1/2} w_{j,n-1} + (\kappa^{n-1/2} + \kappa^{n+1/2}) w_{j,n} - \kappa^{n+1/2} w_{j,n+1}, & j > n, \\ \kappa^{n+1/2} - \kappa^{n-1/2} [2^{1-\alpha} - 2], & j = n. \end{cases}$$

3.2 Existence and uniqueness

Following the same path as in section (2.2), we now study the existence and uniqueness of the finite difference solution U^n for the proposed scheme in equation (17).

As in the case of the LS fractional derivative, the existence of the finite difference solution to the RS scheme follows from its uniqueness, and it is sufficient to show that the finite difference solution U is identically zero when $f^n = 0$ for $n = 1, \dots, P-1$. To do so, we proceed by multiplying both sides of (18) by U^n and summing over the index n , to get

$$\sum_{n=1}^P U^n \kappa^{n-1/2} \sum_{j=n}^P w_{j,n} \delta U^j - \sum_{n=1}^{P-1} U^n \kappa^{n+1/2} \sum_{j=n+1}^P w_{j,n+1} \delta U^j = 0.$$

Using $U^0 = 0$ we have

$$\sum_{n=2}^P U^{n-1} \kappa^{n-1/2} \sum_{j=n}^P w_{j,n} \delta U^j = \sum_{n=1}^P U^{n-1} \kappa^{n-1/2} \sum_{j=n}^P w_{j,n} \delta U^j,$$

and it ensues that

$$\sum_{n=1}^P \kappa^{n-1/2} \delta U^n \sum_{j=n}^P w_{j,n} \delta U^j = 0.$$

Changing the summation order and swapping the indexes leads to:

$$\sum_{n=1}^P \delta U^n \sum_{j=1}^n w_{n,j} \kappa^{j-1/2} \delta U^j = 0.$$

This equation can be cast in the matrix form,

$$\Phi \mathbf{W}_\alpha \mathbf{A} \Phi^T = \mathbf{0}, \quad (19)$$

with the same matrices \mathbf{W}_α and \mathbf{A} as in equation (14). It is again immediate to show that $\mathbf{W}_\alpha \mathbf{A}$ is a positive definite matrix, such that the unique solution of (19) is $\Phi \equiv \mathbf{0}$. Consequently, the finite difference solution $U^n = 0$ for $1 \leq n \leq P-1$ because $U^0 = U^P = 0$. This completes the proof of the existence and uniqueness of the finite difference solution U .

3.3 Truncation error

Next, we study the truncation error T_h^n of the proposed finite difference discretization of problem (16). As in the case of LS fractional derivative ($\theta = 1$), we assume that $f \in C^1(\bar{\Omega})$, $\kappa \in C^2(\bar{\Omega})$ and $u \in C^3(\bar{\Omega})$.

From (16) and (17), the truncation error is in this case

$$T_h^n = \partial_x(\kappa_x D_b^\alpha u)(x_n) - Q_h^n$$

where

$$Q_h^n = \frac{1}{h^2} \left(\kappa^{n+1/2} ({}_x I_b^{1-\alpha} \delta u)(x_n) - \kappa^{n-1/2} ({}_x I_b^{1-\alpha} \delta u)(x_{n-1}) \right)$$

is the proposed finite difference approximation of the RS operator. Regarding the continuous part, we proceed with a procedure similar to the LS case, to get

$$h \partial_x(\kappa_x D_b^\alpha u)(x_n) = \int_{I_n} f^n dx = \int_{I_n} [f(x_n) - f(x)] dx + \int_{I_n} \partial_x(\kappa_x D_b^\alpha u)(x) dx.$$

For the first integral, we have

$$\int_{I_n} [f(x_n) - f(x)] dx = h^2 f'(\zeta_n), \quad \text{for some } \zeta_n \in I_n.$$

For the second integral, we define

$$\int_{I_n} \partial_x(\kappa_x D_b^\alpha u)(x) dx = \kappa^n {}_x I_b^{1-\alpha} u'(x_n) - \kappa^{n-1} {}_x I_b^{1-\alpha} u'(x_{n-1}) := G_h^n,$$

to get the intermediate result

$$T_h^n = O(h) + G_h^n - Q_h^n.$$

The treatment of the remaining contributions relies on the change of variable $s = q - h$ to derive the following two expressions,

$$\begin{aligned} {}_x I_b^{1-\alpha} u'(x_{n-1}) &= \sum_{j=n}^P \int_{I_j} \omega_{1-\alpha}(s - x_{n-1}) u'(s) ds \\ &= \int_{I_P} \omega_{1-\alpha}(s - x_{n-1}) u'(s) ds + \sum_{j=n+1}^P \int_{I_j} \omega_{1-\alpha}(q - x_n) u'(q - h) dq, \end{aligned} \quad (20)$$

and

$$\begin{aligned}
{}_x I_b^{1-\alpha} \delta u(x_{n-1}) &= \sum_{j=n}^P \int_{I_j} \omega_{1-\alpha}(s - x_{n-1}) \delta u^j ds \\
&= \delta u^P \int_{I_P} \omega_{1-\alpha}(s - x_{n-1}) ds + \sum_{j=n+1}^P \delta u^{j-1} \int_{I_j} \omega_{1-\alpha}(q - x_n) dq.
\end{aligned} \tag{21}$$

On the one hand, the equality in (21) is used to obtain

$$h^2 Q_h^n = \kappa^{n-1/2} u^{P-1} \int_{I_P} \omega_{1-\alpha}(s - x_{n-1}) ds + \sum_{j=n+1}^P [\kappa^{n+1/2} \delta u^j - \kappa^{n-1/2} \delta u^{j-1}] \int_{I_j} \omega_{1-\alpha}(s - x_n) ds,$$

where for the second sum, one shows that

$$\begin{aligned}
\kappa^{n+1/2} \delta u^j - \kappa^{n-1/2} \delta u^{j-1} &= [(\kappa^{n+1/2} - \kappa^n) + \kappa^n][\delta u^j - \delta u^{j-1}] + [\kappa^{n+1/2} - \kappa^{n-1/2}] \delta u^{j-1} \\
&= h^2 \left[\frac{h}{2} \kappa'(x_n) + \kappa^n \right] u''(x_{j-1}) + h^2 \kappa'(x_n) u'(x_{j-1}) + O(h^3) \\
&= \frac{h^3}{2} \kappa'(x_n) u''(x_{j-1}) + h^2 \kappa^n [u''(q-h) + (u''(x_{j-1}) - u''(q-h))] \\
&\quad + h^2 \kappa'(x_n) [u'(q-h) + (u'(x_{j-1}) - u'(q-h))] + O(h^3) \\
&= h^2 \kappa^n u''(q-h) + h^2 \kappa'(x_n) u'(q) + O(h^3),
\end{aligned}$$

for any $q \in (x_{j-1}, x_j)$. On the other hand, using equation (20) we have

$$h G_h^n = \sum_{j=n+1}^P \int_{I_j} \omega_{1-\alpha}(q - x_n) [\kappa^n u'(q) - \kappa^{n-1} u'(q-h)] dq - \kappa^{n-1} \int_{I_P} \omega_{1-\alpha}(s - x_{n-1}) u'(s) ds,$$

where, by Taylor series expansion,

$$\begin{aligned}
\kappa^n u'(q) - \kappa^{n-1} u'(q-h) &= \kappa^n [u'(q) - u'(q-h)] + [\kappa^n - \kappa^{n-1}] u'(q-h) \\
&= h \kappa^n u''(q-h) + h \kappa'(x_n) u'(q-h) + O(h^2).
\end{aligned}$$

Combining the above estimates, we obtain for $1 \leq n \leq P-1$

$$T_h^n = E^n + O(h), \quad E^n := -h^{-2} \int_{I_P} \omega_{1-\alpha}(s - x_{n-1}) [h \kappa^{n-1} u'(s) + \kappa^{n-1/2} u^{P-1}] ds.$$

Since

$$\kappa^{n-1/2} u^{P-1} = [\kappa^{n-1} + O(h)] [-h u'(x_{P-1}) + O(h^2)] = -h \kappa^{n-1} u'(s) + O(h^2),$$

$$E^n = O(1) \int_{I_P} \omega_{1-\alpha}(s - x_{n-1}) ds = O(h) \omega_{1-\alpha}(\xi - x_{n-1}), \quad \text{for some } \xi \in I_P.$$

Therefore, for $0 < \alpha < 1$, the truncation error is of order h for x_n not close to the boundary $x = b$.

4 Two-sided fractional derivative

In this section, we return to the two-sided fractional differential equation (1). To construct our finite difference approximation we simply combine the finite difference schemes introduced in the two previous sections for the LS and RS fractional derivatives. Specifically, using (9) and (17), the finite difference solution $U^n \approx u^n$ of the fractional model problem (1) is given by the equations

$$\begin{aligned}
\kappa^{n-1/2} [\theta {}_a I_x^{1-\alpha} \partial U(x_n) + (1-\theta) {}_x I_b^{1-\alpha} \partial U(x_{n-1})] \\
- \kappa^{n+1/2} [\theta {}_a I_x^{1-\alpha} \partial U(x_{n+1}) + (1-\theta) {}_x I_b^{1-\alpha} \partial U(x_n)] = h^2 f^n,
\end{aligned}$$

for $n = 1, \dots, P-1$, and $U^0 = U^P = 0$.

The finite difference solution is obtained by solving the linear system $\mathbf{B}\mathbf{U} = \mathbf{F}$, where $\mathbf{B} = \theta\mathbf{B}_L + (1-\theta)\mathbf{B}_R$, with the definitions of the matrices \mathbf{B}_L and \mathbf{B}_R given in the previous sections. For instance, for $\theta = 1/2$ we get

$$\mathbf{B} = \frac{1}{2} \begin{bmatrix} \ell_{1,1} & \ell_{1,2} & d_{1,3} & d_{1,4} & d_{1,5} & \cdots & d_{1,P-1} \\ \ell_{2,1} & \ell_{2,2} & \ell_{2,3} & d_{2,4} & d_{2,5} & \cdots & d_{2,P-1} \\ c_{3,1} & \ell_{3,2} & \ell_{3,3} & \ell_{3,4} & d_{3,5} & \cdots & d_{3,P-1} \\ c_{4,1} & c_{4,2} & \ell_{4,3} & \ell_{4,4} & \ell_{4,5} & \cdots & b_{4,P-1} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \cdots & \vdots \\ c_{P-1,1} & c_{P-1,2} & c_{P-1,3} & c_{P-1,4} & \cdots & \ell_{P-1,P-2} & \ell_{P-1,P-1} \end{bmatrix}$$

where

$$\begin{aligned} \ell_{i,i} &= c_{i,i} + d_{i,i} = (\kappa^{i-1/2} + \kappa^{i+1/2})[3 - 2^{1-\alpha}] \\ \ell_{i+1,i} &= c_{i+1,i} + d_{i+1,i} = \kappa^{i+1/2}[2^{1-\alpha} - 3] - \kappa^{i+3/2}[3^{1-\alpha} - 2^{2-\alpha} + 1], \\ \ell_{i,i+1} &= c_{i,i+1} + d_{i,i+1} = \kappa^{i+1/2}[2^{1-\alpha} - 3] - \kappa^{i-1/2}[3^{1-\alpha} - 2^{2-\alpha} + 1]. \end{aligned}$$

This shows that the numerical scheme amounts to inverting a full system of $(P-1)$ linear equations in the $P-1$ unknowns, so the existence of the finite difference solution follows from its uniqueness. Following a similar path as for the proof of uniqueness for the cases of the LS and RS fractional derivative schemes (see (14) and (19)), we obtain

$$\Phi[\theta\mathbf{A}\mathbf{W}_\alpha + (1-\theta)\mathbf{W}_\alpha\mathbf{A}]\Phi^T = \mathbf{0}. \quad (22)$$

Since both $\mathbf{A}\mathbf{W}_\alpha$ and $\mathbf{W}_\alpha\mathbf{A}$ are positive definite matrices, Eq. (22) implies $\Phi \equiv \mathbf{0}$ for any $0 \leq \theta \leq 1$, and it follows that $U^n = 0$ for $1 \leq n \leq P-1$ because $U^1 = U^P = 0$. This completes the proof of the existence and uniqueness of the finite difference solution U .

Furthermore, by combining the results of sections 2 and 3, it is trivial to show that the truncation error is of order $O(h)$ (not near the boundaries at $x = a, b$), provided that the regularity conditions on κ , f and u stated in subsections 2.3 and 3.3 are met.

5 Numerical results

In this section we present several numerical experiments to support the theoretical analyses of the previous sections. Specifically, we consider the model problem in (1) over $\Omega = (0, 1)$, subject to homogeneous Dirichlet (absorbing) boundary conditions, and we set $\kappa = 1 + \exp(x)$. The finite difference discretization uses uniform spatial meshes with $P = 2^l$ subintervals, for $l > 1$, such that $h = 1/P$. The solution error E_h is measured using the discrete L^∞ -norm $\|v\|_h = \max_{0 \leq i \leq P} |v(x_i)|$. Based on this error definition, the numerical estimate of convergence rates σ_h of the finite difference solutions is obtained from the relation $\sigma_h = \log_2(E_{2h}/E_h)$.

5.1 Example 1: smooth solutions

We first consider the source term f leading to the exact solution

$$u_{\text{ex}}(x) = x^{4-\theta(1-\alpha)}(1-x)^{4-(1-\theta)(1-\alpha)}. \quad (23)$$

The determination of the source term f corresponding to u_{ex} is detailed in Appendix A.

We first fix $\theta = 1/2$, $P = 4192$ and report in Figure 1 the estimates σ_h as a function of α . The plot shows that $\sigma_h \sim 1$, denoting an error in $O(h)$, for almost all values of α except in the immediate neighborhood of $\alpha = 1$. When $\alpha \rightarrow 1$, σ_h exhibits a rapidly varying behavior to reach the expected second order convergence rate (error in $O(h^2)$) at $\alpha = 1$.

Next, we fix $P = 512$ and plot the L^∞ -norm of E_h against α for different values of θ . Results are reported in Figure 2. We observe that the errors are almost the same for $\theta = 0.25$ and $\theta = 0.75$, and for

Table 1: Discrete L^∞ -norm errors E_h and estimated numerical convergence rates σ_h for different values of α , θ and spatial discretization step size h .

| θ | $-\log_2 h$ | $\alpha = 0.25$ | | $\alpha = 0.50$ | | $\alpha = 0.75$ | |
|----------|-------------|-----------------|------------|-----------------|------------|-----------------|------------|
| | | E_h | σ_h | E_h | σ_h | E_h | σ_h |
| 0.0 | 6 | 2.069e-04 | 0.9877 | 1.568e-04 | 0.9493 | 9.656e-05 | 0.8750 |
| | 7 | 1.040e-04 | 0.9929 | 8.028e-05 | 0.9659 | 5.164e-05 | 0.9030 |
| | 8 | 5.214e-05 | 0.9960 | 4.080e-05 | 0.9765 | 2.723e-05 | 0.9234 |
| | 9 | 2.611e-05 | 0.9976 | 2.064e-05 | 0.9834 | 1.421e-05 | 0.9382 |
| | 10 | 1.307e-05 | 0.9986 | 1.040e-05 | 0.9882 | 7.357e-06 | 0.9496 |
| 0.25 | 6 | 3.528e-04 | 0.9535 | 1.876e-04 | 0.9239 | 8.120e-05 | 0.8739 |
| | 7 | 1.784e-04 | 0.9838 | 9.622e-05 | 0.9636 | 4.275e-05 | 0.9255 |
| | 8 | 8.875e-05 | 1.0071 | 4.843e-05 | 0.9905 | 2.200e-05 | 0.9588 |
| | 9 | 4.325e-05 | 1.0369 | 2.393e-05 | 1.0173 | 1.108e-05 | 0.9887 |
| | 10 | 2.033e-05 | 1.0894 | 1.150e-05 | 1.0569 | 5.432e-06 | 1.0290 |
| 0.5 | 6 | 5.451e-04 | 0.8593 | 2.024e-04 | 0.8990 | 7.127e-05 | 8.7540 |
| | 7 | 2.865e-04 | 0.9280 | 1.045e-04 | 0.9530 | 3.705e-05 | 9.4381 |
| | 8 | 1.461e-04 | 0.9713 | 5.269e-05 | 0.9883 | 1.868e-05 | 9.8776 |
| | 9 | 7.289e-05 | 1.0036 | 2.599e-05 | 1.0198 | 9.157e-06 | 1.0287 |
| | 10 | 3.545e-05 | 1.0398 | 1.243e-05 | 1.0643 | 4.304e-06 | 1.0893 |
| 0.75 | 6 | 3.353e-04 | 0.9282 | 1.818e-04 | 0.9071 | 7.899e-05 | 0.8529 |
| | 7 | 1.714e-04 | 0.9672 | 9.392e-05 | 0.9527 | 4.190e-05 | 0.9147 |
| | 8 | 8.632e-05 | 0.9898 | 4.757e-05 | 0.9812 | 2.167e-05 | 0.9513 |
| | 9 | 4.289e-05 | 1.0092 | 2.370e-05 | 1.0054 | 1.097e-05 | 0.9820 |
| | 10 | 2.094e-05 | 1.0341 | 1.156e-05 | 1.0359 | 5.408e-06 | 1.0205 |
| 1.0 | 6 | 2.047e-04 | 0.9728 | 1.537e-04 | 0.9289 | 9.350e-05 | 0.8512 |
| | 7 | 1.034e-04 | 0.9855 | 7.929e-05 | 0.9546 | 5.048e-05 | 0.8893 |
| | 8 | 5.197e-05 | 0.9922 | 4.048e-05 | 0.9700 | 2.677e-05 | 0.9149 |
| | 9 | 2.607e-05 | 0.9956 | 2.053e-05 | 0.9794 | 1.403e-05 | 0.9326 |
| | 10 | 1.306e-05 | 0.9975 | 1.037e-05 | 0.9857 | 7.283e-06 | 0.9457 |

$\theta = 0$ and $\theta = 1$. This is due to the similar singularity behavior near the boundaries of the exact solution u_{ex} in (23) for any choice of $\theta = c$ and $\theta = 1 - c$. Note that the errors are decreasing as $\alpha \rightarrow 1$ for all θ . Interestingly enough, Figure 2 also shows that for $\alpha < 0.6$, the error is lower for extreme values of θ , that is close to 0 or 1, and on the contrary E_h is lower for intermediate values ($\theta \approx 1/2$) when $\alpha > 0.6$.

Table 1 reports the L^∞ -norm of E_h and the corresponding estimates of convergence rate for different values of α , θ and the discretization step size h . The table confirms the $O(h)$ errors, for all the values of α and θ shown, as h goes to zero.

5.2 Example 2: non-smooth solutions

In practice, due to the presence of the two-sided fractional derivative, the solution u of (1) admits end-point singularities even if the source term f is smooth. It was proved recently in [17] that, for $\theta = 1/2$, the leading singularity term takes the form $x^{\frac{1+\alpha}{2}}(1-x)^{\frac{1+\alpha}{2}}$ when the diffusivity coefficient κ is constant. Similarly, one can show that leading singularity term takes the form $(x-a)^\alpha$, with

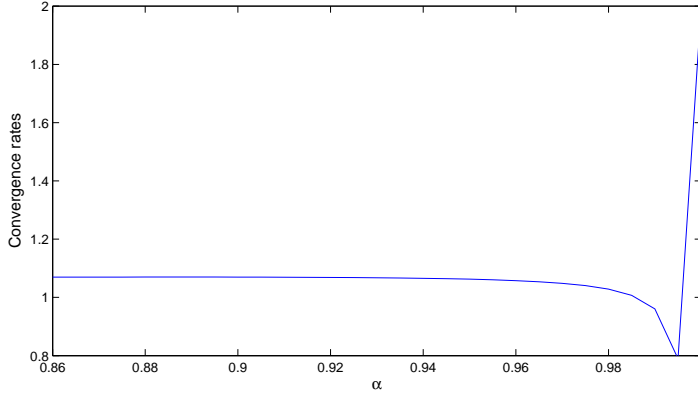


Figure 1: Graphical plot of the numerical convergence rates σ_h against the diffusion exponent α . Computations use $\theta = 1/2$ and $P = 4192$.

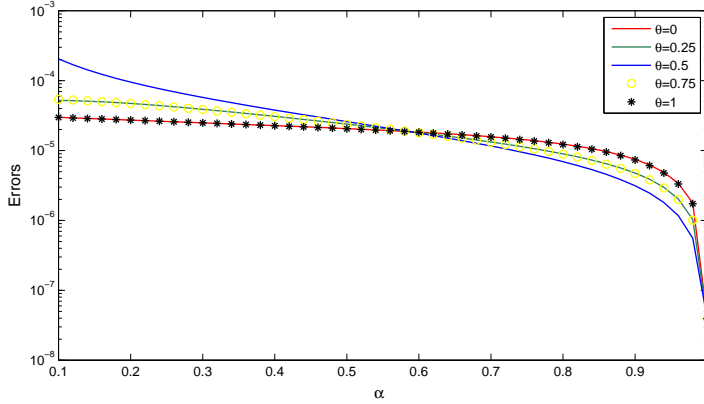


Figure 2: Discrete L^∞ -norm of error E_h against the diffusion exponent α , for $P = 512$ and different values of θ as indicated.

$a = 0$ presently, in the case of LS fractional derivative ($\theta = 1$), and the form $(b - x)^\alpha$, with $b = 1$ presently, in the case of RS fractional derivatives ($\theta = 0$). For smooth κ , we conjecture the same singular behavior. Furthermore, we suggest that for $0 \leq \theta \leq 1$, the leading singularity term has the generic form $(x - a)^{1-\theta(1-\alpha)}(b - x)^{1-(1-\theta)(1-\alpha)}$ ($a = 0$ and $b = 1$ in the present example). However, demonstrating this point remains an open problem and it will be a subject of future work.

To support our claim, we choose now the source term f such that $u_{\text{ex}}(x) = x^{1-\theta(1-\alpha)}(1-x)^{1-(1-\theta)(1-\alpha)}$ is the exact solution of the problem with other settings as before. One can easily check that the truncation errors analyses provided above are not valid in this situation. We then apply to this problem our finite difference scheme for the LS ($\theta = 1$) and RS ($\theta = 0$) fractional derivatives cases for different values of α and h . Table 2 reports the discrete L^∞ -norm of E_h and estimates of the convergence rates σ_h . The results clearly indicate a convergence rate of the error in $O(h^\alpha)$.

This degradation of the convergence rate was expected because the low regularity of the solution: $u_{\text{ex}} \in C^\alpha[0, 1]$. In the context of time-stepping schemes for fractional diffusion of fractional wave equations, adapted meshes with refinement (clustering of elements) around the singularity successfully improve the errors and consequently, the convergence rates, see [18, 20]. To check if such refinement approach could be useful in our problem of (steady) spatial fractional diffusion problem, we set $\theta = 1$ (LS singularity) and consider a family of graded spatial meshes of $\Omega = (0, 1)$ based on a sequence of points given by

Table 2: Discrete L^∞ -norm errors E_h and estimated numerical convergence rates σ_h for different values of α , θ and spatial discretization step size h .

| θ | $-\log_2 h$ | $\alpha = 0.25$ | | $\alpha = 0.50$ | | $\alpha = 0.75$ | |
|----------|-------------|-----------------|------------|-----------------|------------|-----------------|------------|
| | | E_h | σ_h | E_h | σ_h | E_h | σ_h |
| 0.0 | 7 | 5.057e-02 | 0.2752 | 1.916e-02 | 0.5123 | 4.624e-03 | 0.7626 |
| | 8 | 4.214e-02 | 0.2632 | 1.348e-02 | 0.5068 | 2.732e-03 | 0.7590 |
| | 9 | 3.527e-02 | 0.2567 | 9.510e-03 | 0.5037 | 1.618e-03 | 0.7556 |
| | 10 | 2.959e-02 | 0.2534 | 6.716e-03 | 0.5019 | 9.601e-04 | 0.7533 |
| | 11 | 2.485e-02 | 0.2517 | 4.745e-03 | 0.5010 | 5.702e-04 | 0.7518 |
| | 12 | 2.088e-02 | 0.2509 | 3.354e-03 | 0.5005 | 3.388e-04 | 0.7510 |
| 1.0 | 7 | 4.895e-02 | 0.2297 | 1.881e-02 | 0.4877 | 4.496e-03 | 0.7289 |
| | 8 | 4.145e-02 | 0.2399 | 1.336e-02 | 0.4940 | 2.692e-03 | 0.7402 |
| | 9 | 3.498e-02 | 0.2449 | 9.465e-03 | 0.4970 | 1.606e-03 | 0.7454 |
| | 10 | 2.946e-02 | 0.2475 | 6.700e-03 | 0.4985 | 9.562e-04 | 0.7478 |
| | 11 | 2.480e-02 | 0.2487 | 4.740e-03 | 0.4993 | 5.690e-04 | 0.7490 |
| | 12 | 2.086e-02 | 0.2494 | 3.352e-03 | 0.4996 | 3.384e-04 | 0.7495 |

$x_i = (i/P)^\gamma$, $i = 0, \dots, P$ and $\gamma \geq 1$ is a refinement parameter. The objective is to refine the mesh at the boundary $x = 0$ where the solution has a singularity. Table 3 reports the evolution with $\log_2(P)$ of the L^∞ -norm of the error and estimated convergence rate σ_h and using $\gamma = 2, 3$ and 4. The results show that one can obtain a convergence rate of the error that is $O(h^{\alpha\gamma})$. Finally, Figure 3 compares the pointwise errors obtained for uniform and non-uniform meshes with $\gamma = 3$ when using the same number of discretization points $P = 256, 512, 1024$ and 2048. The reduction of the error due to the mesh refinement is clearly visible. Note that similar results can be obtained for $\theta = 0$ using discretization points defined by $x_i = 1 - ((P - i)/P)^\gamma$ to refine the mesh at the endpoint $x = 1$.

Table 3: Discrete L^∞ -norm errors E_h and estimated numerical convergence rates σ_h for $\alpha = 0.25$, $\theta = 1$ (LS fractional derivatives), different number of discretization points (P) and refinement parameters γ .

| $\log_2 P$ | $\gamma = 2$ | | $\gamma = 3$ | | $\gamma = 4$ | |
|------------|--------------|------------|--------------|------------|--------------|------------|
| | E_h | σ_h | E_h | σ_h | E_h | σ_h |
| 6 | 2.300e-02 | | 8.128e-03 | | 2.871e-03 | |
| 7 | 1.628e-02 | 0.4988 | 4.838e-03 | 0.7484 | 1.438e-03 | 0.9976 |
| 8 | 1.151e-02 | 0.4996 | 2.878e-03 | 0.7495 | 7.194e-04 | 0.9992 |
| 9 | 8.140e-03 | 0.4998 | 1.711e-03 | 0.7498 | 3.597e-04 | 0.9997 |
| 10 | 5.756e-03 | 0.4999 | 1.018e-03 | 0.7499 | 1.800e-04 | 0.9999 |
| 11 | 4.070e-03 | 0.4999 | 6.051e-04 | 0.7499 | 8.994e-05 | 0.9999 |
| 12 | 2.878e-03 | 0.5002 | 3.600e-04 | 0.7500 | 4.497e-05 | 0.9998 |

6 Concluding remarks

The objective of this work was to propose and analyze a finite-difference scheme for the solution of general one-dimensional fractional elliptic problems with a variable diffusion coefficient. For the proposed scheme,

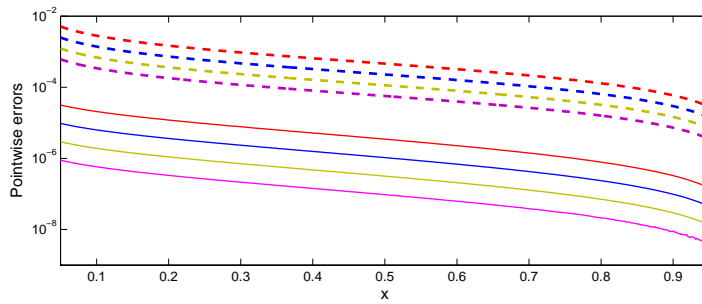


Figure 3: Pointwise errors using uniform (dashed lines) and nonuniform meshes with $\gamma = 3$ (solid lines), for $\theta = 0.25$ with $P = 256, 512, 1024, 2048$ (in order from top to bottom).

we proved the existence and uniqueness of the numerical solution and established the order of convergence for the truncation error with the spatial step size. Some numerical results were also presented for problems admitting both smooth and nonsmooth solutions.

This paper will form a stepping stone for the researchers who are interested in computational solutions of variable coefficient two-sided fractional derivative problems. The results obtained in this work lead to several questions that will have to be addressed in the future. First, it will be crucial to address the reason(s) for the dramatic deterioration in the order of convergence of the finite difference scheme when the fractional order α immediately departs from 1 (classical case)? Second, it will be interesting to explore the possibility of incorporating the fractional exponent α directly in the finite difference discretization, that is, fractionalizing the numerical scheme. A possible route along this direction could be inspired by the recent research papers on the fractionalization of the Crank-Nicolson time-scheme for solving time-fractional diffusion equation, see [9]. Finally, mechanisms for determining the order of singularity near the boundaries in the case of variable diffusivity remains to be developed. A possibility could be to look at series solution to (1). These and other related open questions will be the subject of future research.

A Source term derivation

Here we detail the derivation of the source term f corresponding to the exact solution $u_{\text{ex}}(x) = x^\mu(1-x)^\nu$ on $\Omega = (0, 1)$ with $\mu, \nu > 0$. A similar route can be used to derive modifications of f in the case of non-homogeneous Dirichlet boundary conditions. With $\partial_x^{\alpha, \theta} u_{\text{ex}} = \theta {}_0D_x^\alpha u_{\text{ex}} + (1-\theta) {}_xD_1^\alpha u_{\text{ex}}$, the solution u_{ex} and f are related by

$$f(x) = -\partial_x (\kappa(x) \partial_x^{\alpha, \theta} u(x)) = -\kappa'(x) \partial_x^{\alpha, \theta} u(x) - \kappa(x) \partial_x^{\alpha+1, \theta} u(x).$$

It follows that

$${}_0D_x^\alpha u_{\text{ex}} = \int_0^x \frac{(x-z)^{-\alpha}}{\Gamma(1-\alpha)} u'_{\text{ex}}(z) dz = \int_0^x \frac{(x-z)^{-\alpha}}{\Gamma(1-\alpha)} [\mu z^{\mu-1}(1-z)^\nu - \nu z^\mu(1-z)^{\nu-1}] dz.$$

Consequently,

$$\begin{aligned} \int_0^x \frac{(x-z)^{-\alpha}}{\Gamma(1-\alpha)} z^{\mu-1}(1-z)^\nu dz &= \sum_{n=0}^{\infty} (-1)^n \binom{\nu}{n} \int_0^x \frac{(x-z)^{-\alpha}}{\Gamma(1-\alpha)} z^{\mu+n-1} dz \\ &= \sum_{n=0}^{\infty} (-1)^n \binom{\nu}{n} \frac{\Gamma(\mu+n)}{\Gamma(\mu-\alpha+n+1)} x^{\mu-\alpha+n}. \end{aligned}$$

Similar computations give

$$\int_0^x \frac{(x-z)^{-\alpha}}{\Gamma(1-\alpha)} z^\mu(1-z)^{\nu-1} dz = \sum_{n=0}^{\infty} (-1)^n \binom{\nu-1}{n} \frac{\Gamma(\mu+n+1)}{\Gamma(\mu-\alpha+n+2)} x^{\mu-\alpha+n+1}.$$

Therefore, defining

$$F_{\nu,\mu,\alpha}^n(x) = \binom{\nu}{n} \frac{\Gamma(\mu+n)}{\Gamma(\mu-\alpha+n+1)} x^{\mu-\alpha+n},$$

we arrive at

$${}_0D_x^\alpha u_{\text{ex}}(x) = \sum_{n=0}^{\infty} (-1)^n (\mu F_{\nu,\mu,\alpha}^n(x) - \nu F_{\nu-1,\mu+1,\alpha}^n(x)),$$

and

$${}_xD_1^\alpha u_{\text{ex}}(x) = \sum_{n=0}^{\infty} (-1)^n (\mu F_{\mu-1,\nu+1,\alpha}^n(1-x) - \nu F_{\mu,\nu,\alpha}^n(1-x)).$$

These two expressions can be appropriately combined to compute the fractional derivative $\partial_x^{\alpha,\theta} u_{\text{ex}}$ and subsequently the source term f .

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