## ON A LEGENDRE TAU METHOD FOR FRACTIONAL BOUNDARY VALUE PROBLEMS WITH A CAPUTO DERIVATIVE

# Kazufumi Ito<sup>1</sup>, Bangti Jin<sup>2</sup>, Tomoya Takeuchi<sup>3</sup>

## Abstract

In this paper, we revisit a Legendre-tau method for two-point boundary value problems with a Caputo fractional derivative in the leading term, and establish an  $L^2$  error estimate for smooth solutions. Further, we apply the method to the Sturm-Liouville problem. Numerical experiments indicate that for the source problem, it converges steadily at an algebraic rate even for nonsmooth data, and the convergence rate enhances with problem data regularity, whereas for the Sturm-Liouville problem, it always yields excellent convergence for eigenvalue approximations.

MSC 2010: Primary 65N35; Secondary 65N15, 34B10

*Key Words and Phrases*: Caputo fractional derivative, Legendre tau method, error estimates, eigenvalue approximation

#### 1. Introduction

We consider a boundary value problem involving a left-sided Caputo fractional derivative in the leading term. Given a potential  $q \in L^{\infty}(D)$ , D = (0, 1), the problem reads

$$- {}_{0}^{C} D_{x}^{\alpha} u + q u = f \quad \text{in } D, \qquad u(0) = u(1) = 0, \tag{1.1}$$

where  $f \in L^2(D)$ ,  $\alpha \in (1,2)$  is the order of the derivative, and  ${}_0^C D_x^{\alpha} u$  is the left-sided Caputo derivative of order  $\alpha$  defined in (2.3) below. In case of  $\alpha = 2$ ,  ${}_0^C D_x^{\alpha} u$  coincides with the usual second-order derivative u'', and the model (1.1) recovers the classical two-point boundary value problem. We also study the related eigenvalue problem: find u and  $\lambda \in \mathbb{C}$  such that

$$- {}_{0}^{C} D_{x}^{\alpha} u + q u = \lambda u \quad \text{in } D, \qquad u(0) = u(1) = 0.$$
(1.2)

<sup>©</sup> Year Diogenes Co., Sofia

pp. xxx-xxx, DOI: .....

The motivations of the models (1.1) and (1.2) stem from the mathematical modeling of anomalous diffusion, especially superdiffusion, in which the mean squares variance grows faster than that in a Gaussian process. The space fractional derivative admits a micro interpretation as asymmetric Lévy flights. Such phenomena were observed in applications, e.g., geophysical flows and magnetized plasmas [6]. In practice, the derivation is often done for the Riemann-Liouville fractional derivative. We refer readers to [1] for a derivation and physical explanations for solute transport in subsurface flow. However, the Caputo derivative gives a number of distinct features: more regular solution profile [6], mass conservation and physical flux/boundary condition [35, 27].

The accurate simulation of the model (1.1) has received much interest. Amongst existing methods, finite difference methods (FDM) [31, 29, 26] and finite element methods (FEM) [7, 16, 17, 19, 34] are predominant, but mostly for the Riemann-Liouville derivative. The study on the Caputo case is scarce, despite its convenient treatment of boundary conditions. In [30], a FDM was developed for (1.1) with a Robin boundary condition, and convergence rates were provided; see also [11] for a comparative numerical study. Jin et al [16] developed a variational formulation for the Caputo derivative, and showed the convergence of the Galerkin FEM. We also refer to [10] for a new interpretation of the Caputo derivative in Sobolev spaces.

The nonlocality of the fractional derivative leading to almost dense linear systems, and thus poses significant storage challenge. One idea to remedy the challenge is to discretize fractional derivatives with spectral methods. Several spectral methods for fractional differential equations (FDEs) were proposed [22, 23, 12, 25, 3, 8, 32], which we briefly review below.

For the diffusion equation with a Riemann-Liouville derivative in time, Li and Xu [22] developed a first space-time spectral Galerkin method, which is exponentially convergent for smooth solutions, and provided a rigorous convergence analysis; see also [23] for space-time fractional diffusion. Hanert [12] proposed a pseudo-spectral method for discretizing a Caputo derivative in time with Mittag-Leffler functions. Mokhtary and Ghoreishi [25] presented a spectral tau method for initial value problems with a Caputo derivative, and gave  $L^2$  error estimates. Li et al [21] derived recursive formulae based on Legendre, Chebyshev and Jacobi polynomials for approximating the Caputo derivative, and proposed a collocation method for solving initial/boundary value problems. Ford et al [8] developed a spectral collocation method for fractional differential equations. Bhrawy and Al Shomrani [3] described a Legendre tau method for FDEs involving multiple Caputo derivatives with constant coefficients, a Legendre tau method based on Legendre-Gauss-Lobatto quadrature for FDEs with variable coefficients and a collocation method.

In these existing works on the Legendre tau method, rigorous error estimates for FDEs with a Caputo derivative in space are still not available. This is not surprising since the solution theory for such problems is still under development [17], and the analysis of the tau method is known to be challenging even for the classical two point boundary value problems [28]. For problem (1.2), there are very few numerical methods, including a shooting method [18] and a Galerkin FEM [16]; see also [14] for the sectorial property of the Caputo derivative and [13] for the smallest eigenvalue (under a different boundary condition). Jin et al [16] developed a FEM with second-order convergence, and established its (suboptimal) convergence rates. To the best of our knowledge, the Legendre tau method has not been applied to problem (1.2).

In this work we revisit the Legendre tau method [15, 4, 5]. For problem (1.1), it has been considered in [3], but without analysis. The purpose of this study is three-folded. First, we provide rigorous error estimates for problem (1.1) with  $q \equiv 0$ , which is the main theoretical contribution of the work. Second, we present numerical experiments with nonsmooth data. This aspect is important in practice, since solutions to FDEs generally have only limited regularity even for smooth problem data; see [8] for an excellent account on this aspect. Our findings indicate that the method converges steadily at an algebraic rate for problem (1.1). Third, the method is applied to problem (1.2), and it exhibits fast convergence for both smooth and discontinuous potentials. Surprisingly, with a Legendre approximation of order N, about one half of the computed eigenvalues are reliable with an absolute error less than  $10^{-3}$ . In sum, our essential contributions include rigorous error estimates, numerical experiments with nonsmooth data and extension to eigenvalue problems.

The rest of the paper is organized as follows. In Section 2, we describe preliminaries of fractional calculus, especially fractional-order Sobolev spaces. Then in Section 3, we describe the Legendre tau method, and discuss its convergence for the source problem. In Section 4, we present numerical experiments to illustrate the convergence behavior and efficiency of the scheme. Throughout, we use the notation c, with or without a subscript, to denote a generic constant, and it may differ at different occurrences, but it is always independent of the polynomial order N.

## 2. Preliminaries on fractional calculus

In this part, we recall preliminaries on fractional calculus and fractional order Sobolev spaces. We first recall the definitions of Caputo and Riemann-Liouville fractional derivatives. For any positive non-integer real number  $\beta$  with  $n - 1 < \beta < n, n \in \mathbb{N}$ , the (formal) left-sided Caputo fractional derivative of order  $\beta$  is defined by (see, e.g., [20, p. 92])

$${}_{0}^{C}D_{x}^{\beta}\phi = {}_{0}I_{x}^{n-\beta}\left(\frac{d^{n}\phi}{dx^{n}}\right),\tag{2.3}$$

and the (formal) left-sided Riemann-Liouville fractional derivative of order  $\beta$  is defined by [20, pp. 70]:

$${}^{R}_{0}D^{\beta}_{x}\phi = \frac{d^{n}}{dx^{n}} \bigg( {}_{0}I^{n-\beta}_{x}\phi \bigg).$$
(2.4)

Here  ${}_0I_x^{\gamma}$  for  $\gamma > 0$  is the left-sided Riemann-Liouville integral operator of order  $\gamma$  defined by

$$\left({}_{0}I_{x}^{\gamma}\phi\right)(x) = \frac{1}{\Gamma(\gamma)} \int_{0}^{x} (x-t)^{\gamma-1}\phi(t)dt.$$

It satisfies a semigroup property: for  $\gamma, \delta > 0$ , there holds [20, p. 73]

$${}_{0}I_{x}^{\gamma+\delta}\phi = {}_{0}I_{x}^{\gamma}{}_{0}I_{x}^{\delta}\phi, \quad \forall \phi \in L^{2}(D).$$

$$(2.5)$$

The right-sided versions of fractional-order integrals and derivatives are defined analogously by

$$({}_xI_1^{\gamma}\phi)(x) = \frac{1}{\Gamma(\gamma)} \int_x^1 (t-x)^{\gamma-1}\phi(t) dt,$$
$${}_x^C D_1^{\beta}\phi = (-1)^n {}_xI_1^{n-\beta} \left(\frac{d^n\phi}{dx^n}\right), \qquad {}_x^R D_1^{\beta}\phi = (-1)^n \frac{d^n}{dx^n} \left({}_xI_1^{n-\beta}\phi\right).$$

Next we recall some function spaces. For any  $\beta \geq 0$ , we denote  $H^{\beta}(\mathbb{R})$  to be the Sobolev space of order  $\beta$  on  $\mathbb{R}$  with the inner product  $(\phi, \psi)_{H^{\beta}(\mathbb{R})} = \int_{-\infty}^{\infty} (1+|\xi|^2)^{\beta} \widehat{\phi}(\xi) \overline{\widehat{\psi}(\xi)} d\xi$ , where  $\widehat{\phi}$  is the Fourier transform of  $\phi$ , and denote the norm by  $\|\cdot\|_{H^{\beta}(\mathbb{R})}$ . For the unit interval D, we set  $H^{\beta}(D) = \{u|_D : u \in H^{\beta}(\mathbb{R})\}$  with the norm  $\|u\|_{H^{\beta}(D)} = \inf_{v \in H^{\beta}(\mathbb{R}), v|_D = u} \|v\|_{H^{\beta}(\mathbb{R})}$ , and  $\widetilde{H}^{\beta}(D) = \{\phi \in H^{\beta}(\mathbb{R}) : \operatorname{supp} \phi \subset \overline{D}\}$ , and denote by  $H_0^{\beta}(D)$  to be the closure of  $C_0^{\infty}(D)$  by the norm  $\|\cdot\|_{H^{\beta}(D)}$ , and by  $H^{-\beta}(D)$  to be the dual space of  $H_0^{\beta}(D)$ . By [33, Theorem 4.3.2], if  $\beta - 1/2 \notin \mathbb{Z}$ , the space  $\widetilde{H}^{\beta}(D)$ coincides with  $H_0^{\beta}(D)$ . Throughout, we denote by  $\overline{u}$  the zero extension of u, and define  $\widetilde{H}_L^{\beta}(D) = \{\phi \in L^2(D) : \overline{\phi} \in H^{\beta}(-\infty, 0)\}$ , and likewise  $\widetilde{H}_R^{\beta}(D)$ . A function  $\phi \in L^2(D)$  can be identified with an element in  $H^{-\beta}(D)$ , and the duality bracket  $\langle \phi, \psi \rangle_{H^{-\beta}(D), H_0^{\beta}(D)}$  coincides with the  $L^2(D)$  inner product  $(\phi, \psi)_{L^2(D)}$ . Further, we write by  $\|\cdot\|_X \sim \|\cdot\|_Y$  for (semi-)norms of Hilbert spaces X and Y, if the two norms are equivalent.

#### LEGENDRE TAU METHOD FOR FRACTIONAL BVPS

Now we recall a useful change of integration order formula:

$$(_0I_x^\beta\phi,\psi) = (\phi, _xI_1^\beta\psi) \quad \forall \phi, \psi \in L^2(D),$$
(2.6)

the integration by parts formula [20, Lemma 2.7]

and the fundamental theorem of fractional calculus [20, p. 74]

$${}^{R}_{0}D^{\beta}_{x}{}_{0}I^{\beta}_{x}\phi = \phi \quad \forall \phi \in L^{1}(D).$$

$$(2.8)$$

Last we collect several results on fractional-order Sobolev spaces. The proof of (2.9) and (2.10) is well known [22, 16], and hence omitted.

THEOREM 2.1. Let  $\beta \in (0, 1/2)$ ,  $\phi \in C_0^{\infty}(D)$ . We have the following (semi-) norm equivalences:

$$\|\phi\|_{H_0^{\beta}(D)} \sim \|_0^R D_x^{\beta} \phi\|_{L^2(D)} \sim \|_x^R D_1^{\beta} \phi\|_{L^2(D)},$$
(2.9)

$$\|\phi\|_{H_0^{\beta}(D)}^2 \sim ({}_0^R D_x^{2\beta} \phi, \phi)_{L^2(D)} \sim (\phi, {}_x^R D_1^{2\beta} \phi)_{L^2(D)},$$
(2.10)

$$\|\phi\|_{H^{-\beta}(D)} \sim \|_0 I_x^{\beta} \phi\|_{L^2(D)} \sim \|_x I_1^{\beta} \phi\|_{L^2(D)}, \qquad (2.11)$$

$$\|\phi\|_{H^{-\beta}(D)}^2 \sim ({}_0I_x^{2\beta}\phi,\phi)_{L^2(D)} \sim (\phi, {}_xI_1^{2\beta}\phi)_{L^2(D)}.$$
 (2.12)

P r o o f. Note that for  $u \in H_0^{\beta}(D)$ , the two norms  $\|\phi\|_{H_0^{\beta}(D)}$  and  $\|\bar{\phi}\|_{H^{\beta}(\mathbb{R})}$  are equal for  $\beta = 0, 1$ , and thus by interpolation [33] also equivalent for any  $0 < \beta < 1$ . Hence, by duality, for  $\phi \in L^2(D)$ , we have

$$\begin{aligned} \|\bar{\phi}\|_{H^{-\beta}(\mathbb{R})} &= \sup_{\psi \in H^{\beta}(\mathbb{R})} \frac{(\bar{\phi}, \psi)_{L^{2}(\mathbb{R})}}{\|\psi\|_{H^{\beta}(\mathbb{R})}} \geq \sup_{\substack{\psi \in H^{\beta}(\mathbb{R}), \\ \operatorname{supp}(\psi) \subset D}} \frac{(\bar{\phi}, \psi)_{L^{2}(\mathbb{R})}}{\|\psi\|_{H^{\beta}(\mathbb{R})}} \\ &\geq \sup_{\psi \in H^{\beta}_{0}(D)} c \frac{(\phi, \psi)_{L^{2}(D)}}{\|\psi\|_{H^{\beta}_{0}(D)}} = c \|\phi\|_{H^{-\beta}(D)}. \end{aligned}$$
(2.13)

(a) **proof of** (2.11). We only show the case  $\|_0 I_x^{\beta} \cdot \|_{L^2(D)}$  since the other case follows analogously. The proof relies on a duality argument and (2.9). By (2.8) and (2.7), we have

$$\begin{split} \|\phi\|_{H^{-\beta}(D)} &= \sup_{v \in H_0^{\beta}(D)} \frac{\langle \phi, v \rangle}{\|v\|_{H_0^{\beta}(D)}} = \sup_{v \in H_0^{\beta}(D)} \frac{\langle_0 I_x^{\beta} \phi, \frac{R}{2} D_1^{\beta} v \rangle}{\|v\|_{H_0^{\beta}(D)}} \\ &\leq \|_0 I_x^{\beta} \phi\|_{L^2(D)} \sup_{v \in H_0^{\beta}(D)} \frac{\|\frac{R}{2} D_1^{\beta} v\|_{L^2(D)}}{\|v\|_{H_0^{\beta}(D)}} \leq c \|_0 I_x^{\beta} \phi\|_{L^2(D)}. \end{split}$$

For the converse, we first note for  $0 < \beta < 1/2$  and any  $\psi \in L^2(D)$ ,  $v = {}_xI_1^{\beta}\psi \in \widetilde{H}_R^{\beta}(D) = H_0^{\beta}(D)$  [16]. Hence, by the definition of the dual norm, (2.9) and (2.7), we deduce

$$\begin{split} \|_{0}I_{x}^{\beta}\phi\|_{L^{2}(D)} &= \sup_{\psi \in L^{2}(D)} \frac{\langle_{0}I_{x}^{\beta}\phi,\psi\rangle}{\|\psi\|_{L^{2}(D)}} = \sup_{v \in H_{0}^{\beta}(D)} \frac{\langle_{0}I_{x}^{\beta}\phi,\frac{R}{x}D_{1}^{\beta}v\rangle}{\|RD_{1}^{\beta}v\|_{L^{2}(D)}} \\ &= \sup_{v \in H_{0}^{\beta}(D)} \frac{\langle\phi,v\rangle}{\|RD_{1}^{\beta}v\|_{L^{2}(D)}} \le c\|\phi\|_{H^{-\beta}(D)}. \end{split}$$

This show the norm equivalence between  $\|_0 I_x^{\beta} \cdot \|_{L^2(D)}$  and  $\| \cdot \|_{H^{-\beta}(D)}$ . (b) **proof of** (2.12) For  $\phi \in C_0^{\infty}(\mathbb{R})$ , by Plancherel's theorem, we have

$$(\phi, {}_0I_x^{2\beta}\phi)_{L^2(D)} = (\bar{\phi}, {}_{-\infty}I_x^{2\beta}\bar{\phi})_{L^2(\mathbb{R})} = (\widehat{\bar{\phi}}, {}_{-\infty}I_x^{2\beta}\bar{\phi})_{L^2(\mathbb{R})}.$$

Since the Fourier transform of  $_{-\infty}I_x^{2\beta}\phi = \frac{x_+^{2\beta-1}}{\Gamma(2\beta)} * \phi$  is given by (see, e.g., [9])

$$\widehat{\int_{-\infty}I_x^{2\beta}\phi(\xi)} = e^{-\operatorname{sgn}(\xi)\operatorname{i}\pi\beta}|\xi|^{-2\beta}\widehat{\phi},$$

we have

$$(\widehat{\bar{\phi}}, \widehat{-\infty}I_x^{2\beta}\overline{\phi})_{L^2(\mathbb{R})} = \int_{-\infty}^{\infty} e^{-\operatorname{sgn}(\xi)\mathrm{i}\theta} |\xi|^{-2\beta} |\widehat{\bar{\phi}}(\xi)|^2 d\xi,$$

where by a similar argument in part (a), we obtain

$$\int_{-\infty}^{\infty} e^{-\operatorname{sgn}(\xi)\mathrm{i}\theta} |\xi|^{-2\beta} |\widehat{\overline{\phi}}(\xi)|^2 \, d\xi = \cos(\pi\beta) |||\xi|^{-\beta} \widehat{\overline{\phi}}||_{L^2(\mathbb{R})}^2$$

By the inequality  $|\xi|^{-s} \ge (1+|\xi|^2)^{-s/2}$  for  $s \ge 0$  and (2.13), we have

$$(\phi, {}_{0}I_{x}^{2\beta}\phi)_{L^{2}(D)} \ge \cos(\beta\pi) \|\phi\|_{H^{-\beta}(\mathbb{R})} \ge c\cos(\beta\pi) \|\phi\|_{H^{-\beta}(D)}.$$

Meanwhile, by (2.5), (2.6), and (2.11), we deduce

$$\begin{aligned} (\phi, {}_{0}I_{x}^{2\beta}\phi)_{L^{2}(D)} &= ({}_{0}I_{x}^{\beta}\phi, {}_{x}I_{1}^{\beta}\phi)_{L^{2}(D)} \leq \|{}_{0}I_{x}^{\beta}\phi\|_{L^{2}(D)}\|_{x}I_{1}^{\beta}\phi\|_{L^{2}(D)} \\ &\leq c\|\phi\|_{H^{-\beta}(D)}^{2}. \end{aligned}$$

Similarly we can show the equivalence for  $(\phi, {}_xI_1^{2\beta}\phi)_{L^2(D)}$ .

REMARK 2.1. By a density argument, the norm equivalence (2.9) (respectively (2.10)) is valid for  $\phi \in H_0^{\beta}(D)$  (respectively  $\phi \in H_0^{2\beta}(D)$ ), and (2.11) and (2.12) hold for  $\phi \in L^2(D)$ . It is well known that for  $0 < \beta < 1/2$ , the spaces  $H_0^{\beta}(D)$  and  $H^{\beta}(D)$  are equal [24]. This together with (2.9) indicates that the induced norms are equivalent on  $H^{\beta}(D)$  for  $0 < \beta < 1/2$ , and (2.7) holds for  $u, v \in H^{\beta}(D)$ .

#### 3. Legendre tau method

In this part, we describe a Legendre tau method for problems (1.1) and (1.2), and derive an error estimate.

3.1. Legendre-tau method. First, we describe a Legendre tau method [4, 15, 5] for approximating the operator  $\mathcal{A} = - {}_0^C D_x^{\alpha} + q$ , i.e.,

$$\mathcal{A}u = -\frac{1}{\Gamma(2-\alpha)} \int_0^x (x-s)^{1-\alpha} u''(s) ds + qu.$$

We denote the operator  $\mathcal{A}$  with  $q \equiv 0$  by  $\mathcal{A}_0$ . We begin with the concept of tau extension. Let  $L_k(x) = P_k(2x-1)$  be a shifted Legendre polynomial defined on the interval D = [0, 1], with  $P_k$  being the kth Legendre polynomial on the interval [-1, 1]. Let  $P^{N-2}$  denote the  $L^2(D)$  orthogonal projection onto the subspace

$$S_{N-2} = \operatorname{span}(\{L_k\}_{k=0}^{N-2})$$

and denote  $u^{N-2} = P^{N-2}u$ . By the orthogonality of shifted Legendre polynomials, the coefficients  $\{u_k\}_{k=0}^{N-2}$  of  $u^{N-2}$  for a given function  $u \in L^2(D)$  are determined by

$$u_k = \frac{1}{2k+1}(u, L_k)_{L^2(D)}, \quad k = 0, \dots, N-2.$$

The tau extension is defined as follows. Given  $u^{N-2} = \sum_{k=0}^{N-2} u_k L_k \in S_{N-2}$ , we consider the polynomial

$$\widetilde{u}^{N}(x) = u^{N-2}(x) + u_{N-1}L_{N-1}(x) + u_{N}L_{N}(x),$$

where the coefficients  $u_{N-1}$  and  $u_N$  are determined so that the Dirichlet boundary condition  $\tilde{u}^N(0) = \tilde{u}^N(1) = 0$  is satisfied. Since  $L_k(0) = (-1)^k$ and  $L_k(1) = 1$  (cf. Lemma 3.1 below),  $u^{N-1}$  and  $u^N$  are given by

$$u_N = -\sum_{k: \text{ even}} u_k$$
 and  $u_{N-1} = -\sum_{k: \text{ odd}} u_k$  if N is even, (3.14)

and

$$u_N = -\sum_{k: \text{ odd}} u_k$$
 and  $u_{N-1} = -\sum_{k: \text{ even}} u_k$  if N is odd. (3.15)

The polynomial  $\tilde{u}^N$  so defined for  $u^{N-2} \in S_{N-2}$  is called a *tau extension of*  $u^{N-2}$ . The tau extension for  $u \in L^2(D)$  is defined to be the tau extension of the projection  $P^{N-2}u \in S_{N-2}$ , also denoted by  $\tilde{u}^N$  and the map from  $u \in X$  to the extension  $\tilde{u}^N$  is denoted by  $\tau^N(u) := \tilde{u}^N$ .

The Legendre-tau approximation  $\mathcal{A}^N : S_{N-2} \to S_{N-2}$  of the operator  $\mathcal{A}$  is defined by

$$\mathcal{A}^N u^{N-2} = P^{N-2} \mathcal{A} \widetilde{u}^N = -P^{N-2}{}_0 I_x^{2-\alpha} P^{N-2} (\widetilde{u}^N)'' + P^{N-2} (q\widetilde{u}^N).$$

The Legendre-tau approximation of  $\mathcal{A}_0$  is denoted by  $\mathcal{A}_0^N$ . The coefficient of  $\mathcal{A}^N u^{N-2}$  with respect to the basis  $L_j$  for  $j = 0, 1, \ldots, N-$ 2 is given by

$$(\mathcal{A}^{N}u^{N-2})_{j} = \frac{1}{1+2j} \int_{0}^{1} L_{j}(x) \left( -\int_{0}^{x} \frac{(x-s)^{1-\alpha}}{\Gamma(2-\alpha)} (\widetilde{u}^{N})'' ds + q(x)\widetilde{u}^{N}(x) \right) dx.$$

REMARK 3.1. Similarly we can derive the Legendre tau approximation to the adjoint operator  $\mathcal{A}^*$ . First we derive the adjoint of  $\mathcal{A}_0$ : For  $\phi^{N-2} \in$  $S_{N-2}$ , we consider the expansion

$$P^{N-2}\left(\int_{s}^{1} \frac{(x-s)^{1-\alpha}}{\Gamma(2-\alpha)} \phi^{N-2}(x) dx\right) = \sum_{k=0}^{N-2} \beta_k L_k(s).$$

and choose  $\beta_{N-1}$  and  $\beta_N$  by the tau extension. In view of (2.6) and the fact  $(\tilde{u}^N)'' \in S_{N-2}$ , then with  $T_N(s) \equiv \beta_{N-1}L_{N-1}(s) + \beta_N L_N(s)$ 

$$\begin{aligned} (\mathcal{A}_0^N u^{N-2}, \phi^{N-2}) &= \int_0^1 \phi^{N-2}(x) \Big( -\int_0^x \frac{(x-s)^{1-\alpha}}{\Gamma(2-\alpha)} (\widetilde{u}^N)'' ds \Big) dx \\ &= -\int_0^1 (\widetilde{u}^N(s))'' P^{N-2} \int_s^1 \frac{(x-s)^{1-\alpha}}{\Gamma(2-\alpha)} \phi^{N-2}(x) dx ds \\ &= -\int_0^1 (\widetilde{u}^N(s))'' \Big( P^{N-2} \int_s^1 \frac{(x-s)^{1-\alpha}}{\Gamma(2-\alpha)} \phi^{N-2}(x) dx + T_N(s) \Big) ds \\ &= -\int_0^1 u^{N-2}(s) \frac{d^2}{ds^2} \Big( P^{N-2} \int_s^1 \frac{(x-s)^{1-\alpha}}{\Gamma(2-\alpha)} \phi^{N-2}(x) dx + T_N(s) \Big) ds. \end{aligned}$$

Hence,  $(\mathcal{A}^*)^N \in \mathcal{L}(S_{N-2}, S_{N-2})$  is given by

$$(\mathcal{A}^*)^N \phi^{N-2} = -\frac{d^2}{ds^2} \left( P^{N-2} \int_s^1 \frac{(x-s)^{1-\alpha}}{\Gamma(2-\alpha)} \phi^N(x) dx + T_N(s) \right) + P^{N-2}(q(s)\phi^{N-2}).$$

Hence the Legendre-tau method also provides an approximation of  $\mathcal{A}^*$ .

Now we can formulate the Legendre tau approximation of problems (1.1) and (1.2). For problem (1.1), it is to find  $u^{N-2} \in S_{N-2}$  such that

$$\mathcal{A}^{N} u^{N-2} = P^{N-2} f. ag{3.16}$$

Similarly, for (1.2) it is to find  $u^{N-2} \in S_{N-2}$  and  $\lambda^N \in \mathbb{C}$  such that

$$\mathcal{A}^N u^{N-2} = \lambda^N u^{N-2}. \tag{3.17}$$

The efficient implementation of (3.16) and (3.17) are well documented in the literature [21], and hence it is omitted. A preliminary convergence of the scheme (3.16) for the case  $q \equiv 0$  is presented next.

3.2. Convergence rate analysis. In this part we present an analysis of the Legendre tau method for the source problem (1.1) with a zero potential  $q \equiv 0$ . The authors are aware of only a few mathematical studies [4, 28] on the Legendre tau method. Due to the nonlocal nature of the Caputo derivative, the convergence rate analysis in these interesting works does not apply to our scheme directly. We begin with some elementary estimates.

LEMMA 3.1. For  $k \ge 0$ , there holds

$$\begin{aligned} \|L_k\|_{L^2(D)}^2 &= \frac{1}{2k+1}, \quad \|L'_k\|_{L^2(D)}^2 = 2k(k+1), \\ \|L''_k\|_{L^2(D)}^2 &= \frac{2}{3}(k^2+k+3)(k-1)k(k+1)(k+2) \end{aligned}$$

P r o o f. The first identity is well known. Using the Rodrigues formula for shifted Legendre polynomials

$$L_k(x) = \frac{1}{k!} \frac{d^k}{dx^k} x^k (x-1)^k,$$

we deduce directly  $(-1)^k L_k(0) = L_k(1) = 1$ ,  $L'_k(1) = (-1)^{k-1} L'_k(0) = k(k+1)$ ,  $(-1)^k L''_k(0) = L''_k(1) = \frac{1}{2}(k-1)k(k+1)(k+2)$ ,  $(-1)^{k-1} L''_k(0) = L'''_k(1) = \frac{1}{6}(k-2)(k-1)k(k+1)(k+2)(k+3)$ . Then by integration by parts and noting the fact that  $L''_k$  is a polynomial of degree max(k-2,0) and it is orthogonal to  $L_k$ , we deduce

$$||L_k'||_{L^2(D)}^2 = \int_0^1 L_k' L_k' dx = -\int_0^1 L_k'' L_k dx + L_k L_k'|_0^1 = 2k(k+1).$$

Likewise, we deduce the second identity.

The next result recalls the approximation properties of the projection operators  $P^N$  and  $\tau^N$ . The estimate on the tau extension  $\tau^N$  requires fairly restrictive regularity assumption  $u \in H^s(D), s \geq 5$ .

LEMMA 3.2. Let  $s \ge r \ge 0$ . Then for the operators  $P^N$  and  $\tau^N$ , there hold for small  $\epsilon \in (0, 1/2)$ 

$$\begin{split} \|P^{N}u - u\|_{H^{r}(D)} &\leq \begin{cases} cN^{2r-s-1/2} \|u\|_{H^{s}(D)}, & r \geq 1, \\ cN^{3r/2-s} \|u\|_{H^{s}(D)}, & 0 \leq r \leq 1, \\ \|\tau^{N}u - u\|_{H^{r}(D)} &\leq cN^{2r+1/2+3\epsilon/2-s} \|u\|_{H^{s}(D)}, & 1 \leq r \leq 2, \ \forall u \in H^{s}(D) \cap H^{1}_{0}(D), \, s \geq 5. \end{split}$$

P r o o f. The first estimate is well known [2, p. 261]. This estimate and Sobolev embedding theorem yield for  $\epsilon \in (0, 1/6)$ , the approximation  $u^{N-2} = P^{N-2}u$  satisfies

$$|u^{N-2}(0) - u(0)| + |u^{N-2}(1) - u(1)| \le c ||P^{N-2}u - u||_{H^{1/2+\epsilon}(D)} \le c(N-2)^{3/2+3\epsilon/2-s} ||u||_{H^s(D)}.$$

By the defining relations of the tau approximation, i.e., (3.14) and (3.15), we have

$$|u_{N-1}| + |u_N| \le |u^{N-2}(0)| + |u^{N-2}(1)|,$$

and consequently

$$|u_{N-1}| + |u_N| \le c(N-2)^{3/2 + 3\epsilon/2 - s} ||u||_{H^s(D)}.$$

By Lemma 3.1, we deduce for r = 1, 2

$$\begin{aligned} \|\tau^{N}u - u\|_{H^{r}(D)} &\leq \|P^{N-2}u - u\|_{H^{r}(D)} + |u_{N-1}|\|L_{N-1}\|_{H^{r}(D)} \\ &+ |u_{N}|\|L_{N}\|_{H^{r}(D)} \\ &\leq c(N-2)^{2r-s-1/2}\|u\|_{H^{s}(D)} + c(N-2)^{3/2+3\epsilon/2-s}N^{2r-1}\|u\|_{H^{s}(D)} \\ &\leq cN^{2r+1/2+3\epsilon/2-s}\|u\|_{H^{s}(D)}. \end{aligned}$$

The remaining assertion for 1 < r < 2 follows by interpolation [33]. 

Our first result shows the unique solvability and stability of the Legendre tau approximation for  $\mathcal{A}_0$ .

THEOREM 3.1. Let  $f \in H_0^{(2-\alpha)/2}(D)$ . (a) There exists a unique Legendre tau solution of  $\mathcal{A}_0^N u^{N-2} = P^{N-2} f$ . (b) The tau extension  $\widetilde{u}^N$  of the Legendre tau solution  $u^{N-2}$  satisfies

$$\|(\widetilde{u}^N)''\|_{H^{-(2-\alpha)/2}(D)} \le c \|f\|_{H^{(2-\alpha)/2}(D)}.$$
(3.18)

P r o o f. Since the map  $\mathcal{A}_0^N$  is between finite dimensional spaces, it suffices to show its injectivity, i.e., if  $\mathcal{A}_0^N u^{N-2} = 0$  for  $u^{N-2} \in S_{N-2}$ , then  $u^{N-2} = 0$  in  $S_{N-2}$ . Now assume  $P^{N-2}{}_0 I_x^{2-\alpha}(\widetilde{u}^N)'' = 0$ . Then multiplying both sides by  $(\widetilde{u}^N)'' \in S_{N-2}$  and integrating over the domain D yields

$$({}_{0}I_{x}^{2-\alpha}(\widetilde{u}^{N})'',(\widetilde{u}^{N})'')_{L^{2}(D)} = (0,(\widetilde{u}^{N})'')_{L^{2}(D)} = 0.$$

Now the positivity of the form  $(\cdot, {}_{0}I_{x}^{2-\alpha}\cdot)_{L^{2}(D)}$ , cf. Theorem 2.1, implies that  $(\widetilde{u}^N)'' = 0$ . This however together with the boundary condition  $\widetilde{u}^N(0) = \widetilde{u}^N(1) = 0$  yields  $\widetilde{u}^N = 0$  and  $u^{N-2} = 0$ . This shows assertion (a). To show the assertion (b), we note that  $v^{N-2} := (\widetilde{u}^N)''$  satisfies

$$P^{N-2}{}_0I_x^{2-\alpha}P^{N-2}v^{N-2} = P^{N-2}f.$$

#### LEGENDRE TAU METHOD FOR FRACTIONAL BVPS 11

By multiplying both sides by  $v^{N-2} \in S_{N-2}$ , we deduce

$$(v^{N-2}, J^{2-\alpha}v^{N-2})_{L^2(D)} = (v^{N-2}, f)_{L^2(D)}$$
  
 
$$\leq \|v^{N-2}\|_{H^{-(2-\alpha)/2}(D)} \|f\|_{H^{(2-\alpha)/2}(D)}.$$

Here the last inequality follows by

$$\|v^{N-2}\|_{H^{-(2-\alpha)/2}(D)} = \sup_{g} \frac{(v^{N-2}, g)_{L^{2}(D)}}{\|g\|_{H^{(2-\alpha)/2}_{0}(D)}} \ge \frac{(v^{N-2}, f)_{L^{2}(D)}}{\|f\|_{H^{(2-\alpha)/2}_{0}(D)}}.$$

This and Theorem 2.1 imply  $\|v^{N-2}\|_{H^{-(2-\alpha)/2}(D)} \leq c\|f\|_{H^{(2-\alpha)/2}(D)}$ , and thus the desired assertion follows.

The next lemma gives a continuity estimate of  ${}_0I_x^{2\beta}: L^2(D) \to H^{\beta}(D).$ 

LEMMA 3.3. Let 
$$g \in L^2(D)$$
 and  $\beta \in (0, 1/2)$ . Then there holds  
 $\|_0 I_x^{2\beta} g\|_{H^\beta(D)} \leq c \|g\|_{L^2(D)}.$ 

Proof. By Theorem 2.1, we deduce

$$\|_0 I_x^{2\beta} g\|_{H^{\beta}(D)} \le c \|_0^R D_x^{\beta} 0 I_x^{2\beta} g\|_{L^2(D)} = c \|_0 I_x^{\beta} g\|_{L^2(D)},$$

where the last line follows from (2.5) and (2.8). Now the assertion follows by the boundedness of  ${}_{0}I_{x}^{2\beta}$  on  $L^{2}(D)$  [20, p. 72, Lemma 2.1].

The next lemma gives the crucial estimate for the convergence result.

LEMMA 3.4. Let u and  $u^{N-2} \in S_{N-2}$  be the solution to problem (1.1) with q = 0 and problem (3.16), respectively. Then there holds

$$||u^{N-2} - u||_{L^2(D)} \le c ||(\tau^N u - u)''||_{L^2(D)} + ||P^{N-2}u - u||_{L^2(D)}.$$

P r o o f. It follows from the relation  $P^{N-2}\mathcal{A}_0^N P^{N-2} = \mathcal{A}_0^N P^{N-2}$  that  $(\mathcal{A}_0^N)^{-1}P^{N-2}\mathcal{A}_0^N P^{N-2}g = P^{N-2}g$  for  $g \in L^2(D)$ . Hence, we have

$$u^{N-2} - u = (\mathcal{A}_0^N)^{-1} P^{N-2} f - u$$
  
=  $(\mathcal{A}_0^N)^{-1} P^{N-2} (\mathcal{A}_0 - \mathcal{A}_0^N P^{N-2}) u + (P^{N-2} - I) u.$  (3.19)

It remains to bound the first term. Let  $w^{N-2} = (\mathcal{A}_0^N)^{-1} P^{N-2} (\mathcal{A}_0 - \mathcal{A}_0^N P^{N-2}) u \in S_{N-2}$ . By the definitions of  $\mathcal{A}_0^N$  and  $\mathcal{A}_0$ , we deduce

$$P^{N-2}(\mathcal{A}_0 - \mathcal{A}_0^N P^{N-2})u = P^{N-2}{}_0 I_x^{2-\alpha} (\tau^N u - u)''.$$

Hence  $w^{N-2} \in S_{N-2}$  satisfies

$$\mathcal{A}_0^N w^{N-2} = P^{N-2} {}_0 I_x^{2-\alpha} (\tau^N u - u)''.$$

Next we estimate the term on the right hand side. By letting  $\beta := (2-\alpha)/2$ and using Lemma 3.3

$$\|_0 I_x^{2-\alpha} (\tau^N u - u)'' \|_{H^{\beta}(D)} \le c \| (\tau^N u - u)'' \|_{L^2(D)}.$$

Upon invoking Theorem 3.1, the tau approximation  $\widetilde{w}^N$  of  $w^{N-2}$  satisfies

$$\|(\widetilde{w}^N)''\|_{H^{-\beta}(D)} \le c \|(\tau^N u - u)''\|_{L^2(D)}.$$
(3.20)

Using the boundary condition  $\widetilde{w}^N(0) = \widetilde{w}^N(1) = 0$  and the boundedness of  ${}_0I_x^{\gamma}$  on  $L^2(D)$ , we deduce

$$\begin{aligned} \|(\widetilde{w}^{N})'\|_{L^{2}(D)}^{2} &= ((\widetilde{w}^{N})', (\widetilde{w}^{N})')_{L^{2}(D)} = (-(\widetilde{w}^{N})'', \widetilde{w}^{N})_{L^{2}(D)} \\ &\leq \|(\widetilde{w}^{N})''\|_{H^{-\beta}(D)} \|\widetilde{w}^{N}\|_{H^{\beta}(D)} \\ &\leq c \|(\widetilde{w}^{N})''\|_{H^{-\beta}(D)} \|(\widetilde{w}^{N})'\|_{L^{2}(D)}. \end{aligned}$$

Consequently,

$$\|(\widetilde{w}^N)'\|_{L^2(D)} \le c \|(\widetilde{w}^N)''\|_{H^{-\beta}(D)}.$$
(3.21)

This together with Poincaré's inequality and (3.20) yields

$$\|\widetilde{w}^{N}\|_{L^{2}(D)} \leq c \|(\tau^{N}u - u)''\|_{L^{2}(D)}.$$

Further, the  $L^2(D)$  orthogonality of shifted Legendre polynomials implies

$$\begin{aligned} \|\widetilde{w}^{N}\|_{L^{2}(D)}^{2} &= \|w^{N-2}\|_{L^{2}(D)}^{2} + |w_{N-1}|^{2} \|L_{N-1}\|_{L^{2}(D)}^{2} \\ &+ |w_{N}|^{2} \|L_{N}\|_{L^{2}(D)}^{2} \geq \|w^{N-2}\|_{L^{2}(D)}^{2}. \end{aligned}$$

Hence  $||w^{N-2}||_{L^2(D)} \le ||\widetilde{w}^N||_{L^2(D)}$ , and we arrive at the following estimate  $||w^{N-2}||_{L^2(D)} \le c||(\tau^N u - u)''||_{L^2(D)}$ 

The desired estimate now follows by the triangle inequality.

We have the following estimate on the tau-extension  $\tilde{u}^N$  of  $u^{N-2}$ .

COROLLARY 3.1. Let u and  $u^{N-2} \in S_{N-2}$  be the solution to the source problem  $\mathcal{A}_0 u = f$  and its Legendre tau approximation, respectively. Then for the tau extension  $\tilde{u}^N$  of  $u^{N-2}$  there holds

$$\|\widetilde{u}^N - u\|_{L^2(D)} \le c \|(\tau^N u - u)''\|_{L^2(D)} + \|\tau^N u - u\|_{L^2(D)}.$$

P r o o f. By the argument in the proof of Lemma 3.4, we have

$$\begin{split} \widetilde{u}^{N} - u &= \tau^{N} (\mathcal{A}_{0}^{N})^{-1} P^{N-2} (\mathcal{A}_{0} - \mathcal{A}_{0}^{N} P^{N-2}) u + (\tau^{N} P^{N-2} - I) u \\ &= \widetilde{w}^{N} + (\tau^{N} - I) u. \end{split}$$

Now the estimate follows from the triangle inequality and (3.21).

Now we state our main theoretical result: convergence rate of the Legendre tau approximation, which is direct from Lemmas 3.2 and 3.4.

THEOREM 3.2. Let  $f \in H_0^{(2-\alpha)/2}(D)$  and  $q \equiv 0$ , and u and  $u^{N-2} \in S_{N-2}$  be the solutions to (1.1) and (3.16), respectively. Then for  $u \in H^s(D) \cap H_0^1(D)$ ,  $s \geq 5$ , and  $\epsilon \in (0, 1/2)$ , there holds

$$||u - u^{N-2}||_{L^2(D)} \le cN^{9/2 + \epsilon - s}.$$

REMARK 3.2. The error estimate in Theorem 3.2 is suboptimal, in view of the estimate for the  $L^2(D)$  projection. By Corollary 3.1, it holds also for the tau extension  $\tilde{u}^N$  of the approximation  $u^{N-2}$ .

## 4. Numerical experiments and discussions

Now we present numerical results to illustrate the efficiency and accuracy of the Legendre tau method in Section 3 for problems (1.1) and (1.2). All the computations are performed on a desktop with 2.0 GHz CPU and 6.00GB RAM using MATLAB (R2009a). We consider the following three potentials: (i)  $q_1(x) \equiv 0$ , (ii)  $q_2(x) = 20x^3(1-x)e^{-x}$ , and (iii)  $q_3(x) = \chi_{[0,1/2)} - \chi_{[1/2,1]}$ , where  $\chi_S$  denotes the characteristic function of the set S. The numerical experiments focus on nonsmooth problem data, since the case of smooth solutions has been extensively studied. We compute the reference solution using a higher-order Legendre tau approximation.

4.1. Numerical results for source problem. First, we illustrate the method on the source problem (1.1), with a smooth solution.

EXAMPLE 4.1. In this example, we consider problem (1.1) with a source term  $f = \frac{\Gamma(128/17)}{\Gamma(128/17-\alpha)} x^{111/17-\alpha} + (x - x^{111/17})q$ , and the potential q being either  $q_2$  or  $q_3$ . The exact solution u is given by  $u = x - x^{111/17}$ .

The numerical results are shown in Fig. 1. The method converges quickly, irrespective of  $\alpha$  and q, since the true solution u is very smooth. Twenty terms in the Legendre tau approximation can almost reach the machine accuracy. This shows clearly the efficiency and accuracy of the method for problem (1.1) with a smooth solution.

Usually for fractional elliptic problems, the solution u cannot be arbitrarily smooth, even if the source term f is very smooth [16]: for  $f \in \widetilde{H}_L^\beta$ and  $q \in C^\beta(\overline{D}) \cap \widetilde{H}_L^\beta(D)$ , the solution u belongs to  $\widetilde{H}_L^{\alpha+\beta}(D) \cap H_0^{\alpha/2}(D)$ ,



FIGURE 1. Numerical results for example 4.1 with (a)  $q_2$  and (b)  $q_3$ .

and often this is the best regularity. Hence, it is important to test the method with a general problem setup. We illustrate it with one example.

EXAMPLE 4.2. We consider problem (1.1) with  $f = x^{\mu} \sin x$ , for the following three cases:

- (a)  $\mu = 0$ ,  $\alpha = 5/4$ , and different q.
- (b)  $\mu = 0$ ,  $q_2$  or  $q_3$ , and different  $\alpha$  values.
- (c)  $\alpha = 3/2$ ,  $q = q_2$  or  $q_3$ , and different  $\mu$  values.

In example 4.2(a), even for a smooth potential q, the solution u is not very smooth: it contains a leading term  $c_{\alpha}x^{1+\alpha}$  for x close to the origin. The errors for  $q_1$  and  $q_2$  are almost identical since  $q_2$  is smoother than f, and for  $q_3$ , the method converges much slower due to limited solution regularity, cf. Table 1. Nonetheless, for all three potentials, a steady algebraic convergence is observed. Example 4.2(b) examines the influence of the fractional order  $\alpha$ : The solution u becomes more smooth as the order  $\alpha$  increases. This is numerically confirmed: as  $\alpha$  increases from  $\alpha = 5/4$ to  $\alpha = 7/4$ , the convergence rate improves accordingly, cf. Fig. 2. The pickup in the convergence rate agrees with the increase of  $\alpha$ . In example 4.2(c), the exponent  $\mu$  determines the smoothness of f in the space  $\widetilde{H}_L^{\beta}(D)$ : the larger is  $\mu$ , the smoother is the solution u in the space  $\widetilde{H}_L^{\beta}(D)$ , for a smooth q. Since  $q_2$  belongs to  $\widetilde{H}_L^{3+\epsilon}(D)$ , whereas  $q_3$  belongs to only  $\widetilde{H}_L^{\epsilon}(D)$ ,  $\epsilon \in (0, 1/2)$ , the regularity of u is determined by f and q for  $q_2$  and  $q_3$ , respectively. For  $q_2$ , the convergence improves as  $\mu$  increases, whereas for  $q_3$ , the convergence is identical for all three different  $\mu$  values, cf. Fig. 3.

Hence, the Legendre tau method can converge reasonably well for problem (1.1) with nonsmooth problem data.

TABLE 1. The  $L^2$ -error for problem (1.1), with  $f = \sin x$  and  $\alpha = 5/4$ .

N	10	20	30	40	50	60	70	80
$q_1$	5.72e-6	3.22e-7	6.13e-8	1.90e-8	7.72e-9	3.69e-9	1.98e-9	1.15e-9
$q_2$	5.85e-6	3.21e-7	6.13e-8	1.90e-8	7.71e-9	3.69e-9	1.98e-9	1.15e-9
$q_3$	4.18e-4	1.19e-4	5.82e-5	3.50e-5	2.36e-5	1.71e-5	1.29e-5	1.01e-5



FIGURE 2. Numerical methods for example 4.2(b).



FIGURE 3. Numerical methods for example 4.2(c) with  $f = x^{\mu} \sin x$ .

4.2. Numerical results for eigenvalue problem. For the Sturm-Liouville problem, first we consider the case of a zero potential  $q_1 = 0$ , and the numerical results are shown in Fig. 4. Here the error  $e(\lambda_k)$  is measured by  $e(\lambda_k) = |\lambda_k - \lambda_k(N)|$ , where  $\lambda_k(N)$  denotes the kth eigenvalue approximate by the Legendre tau method of order N. The error e for a fixed eigenvalue decreases with the increase of the polynomial order N. It shows a fast convergence and gives a very good approximation even with a fairly small N. In Fig. 4(b), we plot the number of eigenvalues that are correct to the third decimal place, i.e.,  $|\lambda_k - \lambda_k(N)| < 10^{-3}$ , denoted by M, for each Legendre polynomial order N. About one half of them are reliable to this accuracy, showing the accuracy and efficiency of the method. Further, we show the errors of the eigenvalues computed with N = 100 and 150 in Fig. 4(c). The smaller is the eigenvalue, the smaller is the error; and for a wide range of eigenvalues, their errors are comparable to each other.

Next we compare the new method with a piecewise linear FEM [16]. The results are presented in Table 2. The FEM solution is obtained using a mesh with 5120 elements. With only N = 50, the 19th and 20th approximate eigenvalues are correct to the fourth decimal place. The FEM approximations are correct only to the third decimal place, despite the very refined mesh. Due to the low-order convergence of the FEM, there are less than 50 eigenvalues correct to the first decimal place, out of 5119 approximate eigenvalues. The Legendre tau method with N = 150 yields accurate estimate for the first 80 eigenvalues. The FEM with 5120 elements takes 35 seconds, but the Legendre tau method with N = 150 takes only 5 seconds, which shows clearly its efficiency for computing eigenvalue approximations. Although not presented, we note that the observations remain valid for a smooth potential, e.g.  $q_2$ .

TABLE 2. The first twenty eigenvalues for problem (1.2) with the potential  $q_1 \equiv 0$ ,  $\alpha = 7/4$ .

N	50	200	FEM (5120)
1	9.59774287e0	9.59774287e0	9.59774275e0
2	2.59580498e1	2.59580498e1	2.59580498e1
3	5.94945502e1	5.94945503e1	5.94945476e1
4	8.29981244e1	8.29981242e1	8.29981300e1
$^{5,6}$	$1.52686548e2 \pm 1.40992295e1i$	$1.52686547 e 2 {\pm} 1.40992314 e 1 i$	$1.52686561 e 2 \pm 1.40991929 e 1 i$
$^{7,8}$	$2.57672556e2 \pm 4.27793096e1i$	$2.57672553 e 2 {\pm} 4.27793143 e 1 i$	$2.57672610 \mathrm{e}2 {\pm} 4.27792461 \mathrm{e}1\mathrm{i}$
$^{9,10}$	$3.84066744e2 \pm 7.88247425e1i$	$3.84066734 e2 {\pm} 7.88247539 e1 i$	$3.84066889e2 \pm 7.88246203e1i$
$11,\!12$	$5.30749764e2 \pm 1.23398271e2i$	$5.30749741 e 2 {\pm} 1.23398295 e 2 i$	$5.30750080 e2 {\pm} 1.23398061 e2 i$
$13,\!14$	$6.96846590e2 \pm 1.76231751e2i$	$6.96846541 \mathrm{e}2{\pm}1.76231796 \mathrm{e}2\mathrm{i}$	$6.96847191 \mathrm{e}2{\pm}1.76231418 \mathrm{e}2\mathrm{i}$
$15,\!16$	$8.81612150e2 \pm 2.36996717e2i$	$8.81612059e2{\pm}2.36996794e2i$	$8.81613193 e2 {\pm} 2.36996225 e2 i$
$17,\!18$	$1.08441846e3 \pm 3.05412459e2i$	$1.08441830 \mathrm{e}3 {\pm} 3.05412583 \mathrm{e}2\mathrm{i}$	$1.08442015 e3 \pm 3.05411765 e2 i$
19,20	$1.30473055e3 \pm 3.81240768e2i$	$1.30473028 e3 \pm 3.81240959 e2 i$	$1.30473313 e3 {\pm} 3.81239828 e2 i$



FIGURE 4. Numerical results for problem (1.2) with  $q_1 \equiv 0$ , from top to bottom  $\alpha = 5/4$ , 3/2 and 7/4. (a): the error ev.s. polynomial order N; (b): the number M of eigenvalues correct to the third decimal place v.s. N, and (c) the errors for the first 100 eigenvalues with N = 100 and 150.

Last we present the results for the discontinuous potential  $q_3(x)$  in Fig. 5. Then the eigenfunctions have limited Sobolev regularity, and thus a fast convergence is not expected. Surprisingly, a fast convergence of eigenvalue approximations is still observed, and it is only slightly slower than that for a smooth potential, albeit less steady: it suffers from slight oscillations as N increases. The approximations are reasonable for a small N, and the accuracy improves steadily with the increase of the polynomial order N.



FIGURE 5. Numerical results for problem (1.2) with  $q_3$ .

## 5. Concluding remarks

We have revisited a Legendre tau method for a boundary value problem with a Caputo fractional derivative in the leading term. A convergence rate result is provided for the source problem with a smooth solution. It shows a good convergence for both smooth and nonsmooth solutions, which awaits further theoretical justifications. The method was applied to the eigenvalue problem. It can yield exceedingly accurate eigenvalue approximations for both smooth and discontinuous potentials. Hence, the method is promising for fractional boundary value problems.

There are many problems deserving further study. First, the analysis of the scheme remains challenging, especially for the case of a nonzero potential, and the optimal  $L^2$  convergence rate is still missing. Second, the convergence of eigenvalue approximations is always very fast, irrespective of the smoothness of the potential, which awaits theoretical justification.

### Acknowledgements

The work of the second author (B. Jin) is partially supported by NSF-DMS 1319052.

#### References

- D. A. Benson, S. W. Wheatcraft, and M. M. Meerschaert. The fractional-order governing equation of Lévy motion. *Water Resour. Res.*, 36(6):1413–1424, 2000.
- [2] C. Bernardi and Y. Maday. Spectral methods. In Handbook of Numerical Analysis, Vol. V, Handb. Numer. Anal., V, pages 209–485. North-Holland, Amsterdam, 1997.
- [3] A. H. Bhrawy and M. M. Al-Shomrani. A shifted Legendre spectral method for fractional-order multi-point boundary value problems. Adv. Diff. Eq., 2012(1):1–19, 2012.
- [4] C. Canuto, M. Y. Hussaini, A. Quarteroni, and T. A. Zang. Spectral Methods in Fluid Dynamics. Springer-Verlag, New York, 1988.

- [5] C. Canuto, M. Y. Hussaini, A. Quarteroni, and T. A. Zang. Spectral Methods. Springer-Verlag, Berlin, 2006. Fundamentals in Single Domains.
- [6] D. del-Castillo-Negrete, B. A. Carreras, and V. E. Lynch. Front dynamics in reaction-diffusion systems with Levy flights. *Phys. Rev. Lett.*, 91(1):018302, 4 pp., 2003.
- [7] V. J. Ervin and J. P. Roop. Variational formulation for the stationary fractional advection dispersion equation. *Numer. Methods Partial Differential Equations*, 22(3):558–576, 2006.
- [8] N. J. Ford, M. L. Morgado, and M. Rebelo. Nonpolynomial collocation approximation of solutions to fractional differential equations. *Fract. Calc. Appl. Anal.*, 16(4):874–891, 2013.
- [9] I. M. Gel'fand and G. E. Shilov. *Generalized Functions, Vol. I.* Academic Press, New York, 1964.
- [10] R. Gorenflo, Y. Luchko, and M. Yamamoto. Time-fractional diffusion equation in the fractional Sobolev spaces. *Fract. Calc. Appl. Anal.*, 18(3):799–820, 2015.
- [11] J. L. Gracia and M. Stynes. Formal consistency versus actual convergence rates of difference schemes for fractional-derivative boundary value problems. *Fract. Calc. Appl. Anal.*, 18(2):419–436, 2015.
- [12] E. Hanert. On the numerical solution of space-time fractional diffusion models. Comput. Fluids, 46:33–39, 2011.
- [13] J. Henderson and N. Kosmatov. Eigenvalue comparison for fractional boundary value problems with the Caputo derivative. *Fract. Calc. Appl. Anal.*, 17(3):872–880, 2014.
- [14] K. Ito, B. Jin, and T. Takeuchi. On the sectorial property of the Caputo derivative operator. Appl. Math. Lett., 47:43–46, 2015.
- [15] K. Ito and R. Teglas. Legendre-tau approximations for functional-differential equations. SIAM J. Control Optim., 24(4):737–759, 1986.
- [16] B. Jin, R. Lazarov, J. Pasciak, and W. Rundell. Variational formulation of problems involving fractional order differential operators. *Math. Comp.*, 84(296):2665–2700, 2015.
- [17] B. Jin, R. Lazarov, J. Pasciak, and Z. Zhou. Error analysis of a finite element method for the space-fractional parabolic equation. *SIAM J. Numer. Anal.*, 52(5):2272–2294, 2014.
- [18] B. Jin and W. Rundell. An inverse Sturm-Liouville problem with a fractional derivative. J. Comput. Phys., 231(14):4954–4966, 2012.
- [19] B. Jin and Z. Zhou. A singularity reconstructed finite element method for fractional boundary value problems. ESAIM Math. Model. Numer. Anal., 49(5):1261–1283, 2015.
- [20] A. A. Kilbas, H. M. Srivastava, and J. J. Trujillo. Theory and Applications of Fractional Differential Equations. Elsevier, Amsterdam, 2006.
- [21] C. Li, F. Zeng, and F. Liu. Spectral approximations to the fractional integral and derivative. *Fract. Calc. Appl. Anal.*, 15(3):383–406, 2012.
- [22] X. Li and C. Xu. A space-time spectral method for the time fractional diffusion equation. SIAM J. Numer. Anal., 47(3):2108–2131, 2009.
- [23] X. Li and C. Xu. Existence and uniqueness of the weak solution of the space-time fractional diffusion equation and a spectral method approximation. *Commun. Comput. Phys.*, 8(5):1016–1051, 2010.
- [24] J.-L. Lions and E. Magenes. Non-homogeneous Boundary Value Problems and Applications. Vol. I. Springer-Verlag, New York, 1972.

- [25] P. Mokhtary and Ghoreishi. The L2-convergence of the Legendre spectral tau matrix formulation for nonlinear fractional integro differential equations. *Numer. Algor.*, 58:475–496, 2011.
- [26] A. Pedas and E. Tamme. Piecewise polynomial collocation for linear boundary value problems of fractional differential equations. J. Comput. Appl. Math., 236(13):3349– 3359, 2012.
- [27] C. Shen and M. S. Phanikumar. An efficient space-fractional dispersion approximation for stream solute transport modeling. Adv. Water Res., 32(10):1482–1494, 2009.
- [28] J. Shen. A spectral-tau approximation for the Stokes and Navier-Stokes equations. RAIRO Modél. Math. Anal. Numér., 22(4):677–693, 1988.
- [29] E. Sousa. How to approximate the fractional derivative of order 1 < α ≤ 2. Internat. J. Bifur. Chaos Appl. Sci. Engrg., 22(4):1250075, 13, 2012.
- [30] M. Stynes and J. L. Gracia. A finite difference method for a two-point boundary value problem with a Caputo fractional derivative. *IMA J. Numer. Anal.*, 35(2):698–721, 2015.
- [31] C. Tadjeran, M. M. Meerschaert, and H.-P. Scheffler. A second-order accurate numerical approximation for the fractional diffusion equation. J. Comput. Phys., 213(1):205–213, 2006.
- [32] W. Y. Tian, W. Deng, and Y. Wu. Polynomial spectral collocation method for space fractional advection-diffusion equation. *Numer. Methods Partial Differential Equations*, 30(2):514–535, 2014.
- [33] H. Triebel. Interpolation Theory, Function Spaces, Differential Operators. North-Holland Mathematical Library. 1978.
- [34] 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(3):1292–1310, 2014.
- [35] X. Zhang, M. Lv, J. W. Crawford, and I. M. Young. The impact of boundary on the fractional advection-dispersion equation for solute transport in soil: Defining the fractional dispersive flux with the Caputo derivatives. Adv. Water Res., 30(5):1205– 1217, 2007.

<sup>1</sup> Department of Mathematics North Carolina State University Raleigh, NC 27695, USA email: (kito@math.ncsu.edu) Received: February 13, 2015

<sup>2</sup> Department of Computer Science University College London Gower Street, London WC1E 6BT, UK email: (bangti.jin@gmail.com)

<sup>3</sup> Institute of Industrial Science The University of Tokyo Tokyo, Japan email: (takeuchi@sat.t.u-tokyo.ac.jp)