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AN EFFECTIVE ALGORITHM FOR COMPUTING FRACTIONAL DERIVATIVES AND APPLICATION TO FRACTIONAL DIFFERENTIAL EQUATIONS

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Abstract. In recent years, fractional differential equations have been extensively applied to model various complex dynamic systems. The studies on highly accurate and efficient numerical methods for fractional differential equations have become necessary. In this paper, an effective recurrence algorithm for computing both the fractional Riemann-Liouville and Caputo derivatives is proposed, and then spectral collocation methods based on the algorithm are investigated for solving fractional differential equations. By the recurrence method, the numerical stability with respect to N, the number of collocation points, can be improved remarkably in comparison with direct algorithm. Its robustness ensures that a highly accurate spectral collocation method can be applied widely to various fractional differential equations.

Key words. Riemann-Liouville derivative, Caputo fractional derivative, Riesz fractional derivative, spectral collocation method, fractional differentiation matrix.

1. Introduction

Fractional differential equations (FDEs) have been applied widely in many recent studies in applied mathematics, theoretical physics and mechanics, biology, and economics [22, 23, 30, 31]. The fractional derivative is a powerful tool to describe complex systems that have long memory and long-range spatial interactions. In general, however, numerical methods for fractional derivatives and fractional differential equations suffer from heavy costs of computing due to their nature of non-locality. Therefore, numerical study on fractional differential equations by highly accurate and efficient methods is an imperative task. The spectral method, which is suitable for the discretization of the fractional derivative as a global scheme, has begun to draw more and more attentions from scientific researchers [1, 14, 16, 20, 34, 35, 38, 39, 40].

However, one has to overcome two main difficulties for the spectral method dealing with FDEs: one is the computation of fractional derivatives, and the other is the singularity of the solution of FDEs. Indeed, both difficulties are related with the choice of basis functions the spectral method adopted. Today, it is clear that the use of fractional Jacobi functions (also are called the generalized Jacobi functions) as basis functions is more suitable to deal with the singularity of the solution [3, 6, 7, 10, 32, 33]. Nevertheless, the classical polynomial basis is convenient for the computations of FDEs and also to the analysis of spectral approximation [11, 15, 29]. Moreover, using the polynomials as basis function is still highly accurate compared with the other numerical methods, such as finite difference method and finite element method [15]. It is worthwhile to note that some authors engaged in high order methods for the discretization of fractional derivatives, see [17, 18] and the recent works [8, 19] for example.

In this paper, we are concerned with developing an effective algorithm for computing fractional derivatives. The classical polynomials are still adopted here due

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to the consideration that the singularity near boundary can be overcome by the spectral element method based on polynomials, see the recent paper [21] for details. Several recurrence methods are proposed for the computation of the left- and right- Riemann-Liouville fractional derivatives and the left- and right- Caputo fractional derivatives here. Especially, we compare the stability of our method to one of the direct methods [4, 5, 11, 26]. Then, some applications based on the spectral collocation method are presented. Meanwhile, a comparison with the collocation method based on fractional Jacobi functions [32, 33] is performed.

In [15], Li, Zeng and Liu developed a recurrence method to compute fractional integrals and derivatives. Utilizing the three-term recurrence relation and the property of Jacobi polynomials, the authors established a recurrence scheme for the computation of fractional derivatives. In [37] the author presented a spectral/spectral collocation method by using this recurrence method for solving the space fractional diffusion equation. Anyway, the recurrence algorithm is worth further developing for the spectral collocation method due to its high efficiency and accuracy.

We shall take a different route to compute the differentiation matrix in this paper. The main idea comes from the fact that if $f \in P_n^{\alpha,\beta}(x)$, then it implies $\partial_x f \in P_{n-1}^{\alpha+1,\beta+1}(x)$, where $P_n^{\alpha,\beta}(x)$ designates the class of Jacobi polynomials. Therefore, for the Chebyshev polynomials of the first kind with $\alpha = \beta = -\frac{1}{2}$, their derivatives of the first order are the Chebyshev polynomials of the second kind with $\alpha = \beta = \frac{1}{2}$. Thus, some properties of the Chebyshev polynomials of the second kind can be employed, and a simplified and effective recurrence algorithm for the computation of fractional derivatives of the Chebyshev polynomials of the first kind is then derived.

The paper is arranged as follows. In Section 2 we introduce the series expansion of the Jacobi polynomials in detail starting from an eigenvalue problem, and present the direct method for computing the fractional derivatives. The derivations of the recurrence algorithms are presented in Section 3. In Section 4, the fractional differentiation matrices are investigated, and then the approximated errors are proposed, and several examples are presented to illustrate the stability of our method for large polynomial degree. Some applications of our method are considered in Section 5. Here, we mainly consider the multi-term fractional equations, time-space fractional diffusion equations, and the Riesz fractional diffusion equations. We also consider the non-smooth problem, and a comparison with the corrected backward formulae is carried out in this section. Finally, some remarks and conclusions are presented in Section 6.

2. Preliminaries

At first, we recall a fundamental result about the singular eigenvalue problem and some useful analytical formulations of Jacobi polynomials for computation of fractional derivatives(see also [5, 11, 15, 24]). Consider the following eigenvalue problem

$$(w\varphi y_n')'(x) = \lambda_n w(x) y_n(x). \tag{1}$$

where the weight function satisfies the Pearson equation (see [13] for details)

$$(w\varphi)'(x) = w(x)\psi(x)$$

and $\varphi(x) = x^2 + 2rx + s$, $\psi(x) = 2px + q$, and the eigenvalue $\lambda_n = n(n-1+2p)$.

Lemma 2.1 ([12]). *Let $\alpha > -1, \beta > -1$, and r, s, p, q satisfy*

$$2r = -a - b,\ s = ab,\ 2p = \alpha + \beta + 2,\ q = -a(\beta+1) - b(\alpha+1).$$

Then, the following results hold:

i). The eigenvalue problem (1) *has a sequence of solutions of polynomials* y_n *corresponding to* λ_n *which are orthogonal on* (a, b) *with respect to weight* $w(x) = (x-a)^\alpha(b-x)^\beta$*, and satisfy the three-term recurrence relation*

$$\begin{cases} y_0(x) = 1,\ y_1(x) = x - \dfrac{a(\beta+1)+b(\alpha+1)}{\alpha+\beta+2}, \\ y_{n+1}(x) = -\dfrac{n(n+\alpha)(n+\beta)(n+\alpha+\beta)(b-a)^2}{(2n+\alpha+\beta-1)(2n+\alpha+\beta)^2(2n+\alpha+\beta+1)} y_{n-1}(x) \\ \quad + \left\{ x - \dfrac{2n(n+\alpha+\beta+1)(a+b)+[a(\beta+1)+b(\alpha+1)](\alpha+\beta)}{(2n+\alpha+\beta)(2n+\alpha+\beta+2)} \right\} y_n(x). \end{cases}$$

ii). If $(c+a)(c+b) = 0$*, then the solution* $y_n(x)$ *can be written into*

$$y_n(x) = \sum_{k=0}^{n} C_{n,k} \frac{(x+c)^k}{k!},$$

where

$$\begin{aligned} &(n-k)(n+k+\alpha+\beta+1)C_{n,k} = \\ &\qquad - \left[(2k+\alpha+\beta+2)c + (a+b)(k+1) + a\beta + b\alpha\right] C_{n,k+1} \end{aligned}$$

for $k = 0, 1, 2, \cdots, n-1$ *and* $C_{n,n} = n!$. □

Denote by ${}_rF_s(a_1, \cdots, a_r; b_1, \cdots, b_s; z)$ the hypergeometric function defined by

$${}_rF_s(a_1, \cdots, a_r; b_1, \cdots, b_s; z) = \sum_{k=0}^{\infty} \frac{(a_1)_k \cdots (a_r)_k}{(b_1)_k \cdots (b_s)_k} \frac{z^k}{k!},$$

where $(\cdot)_k$ is the Pochhammer symbol defined by

$$(a)_0 = 1,\ (a)_k = \prod_{i=1}^{k} (a+i-1) \text{ for } k = 1, 2, \cdots.$$

Let $P_n^{\alpha,\beta}(x)$ be the Jacobi polynomials corresponding to weight function $w(x) = (1-x)^\alpha(1+x)^\beta$. Then, by their hypergeometric representations [2],

$$P_n^{\alpha,\beta}(x) = \frac{(\alpha+1)_n}{n!} {}_2F_1\left(-n, n+\alpha+\beta+1; \alpha+1; \frac{1-x}{2}\right).$$

Set $a = -1, b = 1$, and let us consider the weight $w(x) = [x-(-1)]^\beta(1-x)^\alpha$, by Lemma 2.1, we derive

$$\begin{aligned} y_n(x) &= \sum_{k=0}^{n} \frac{(-2)^n(\beta+1)_n(-n)_k(n+\alpha+\beta+1)_k}{(n+\alpha+\beta+1)_n(\beta+1)_k} \left(\frac{1}{2}\right)^k \frac{(x+1)^k}{k!} \\ &= \frac{(-2)^n(\beta+1)_n}{(n+\alpha+\beta+1)_n} {}_2F_1\left(-n, n+\alpha+\beta+1; \beta+1; \frac{x+1}{2}\right), \end{aligned} \tag{2}$$

or

$$\begin{aligned} y_n(x) &= \sum_{k=0}^{n} \frac{2^n(\alpha+1)_n(-n)_k(n+\alpha+\beta+1)_k}{(n+\alpha+\beta+1)_n(\alpha+1)_k} \left(-\frac{1}{2}\right)^k \frac{(x-1)^k}{k!} \\ &= \frac{2^n(\alpha+1)_n}{(n+\alpha+\beta+1)_n} {}_2F_1\left(-n, n+\alpha+\beta+1; \alpha+1; -\frac{x-1}{2}\right). \end{aligned} \tag{3}$$

In light of (3) and the hypergeometric representation of $P_n^{\alpha,\beta}(x)$, it follows that

$$y_n(x) = \frac{2^n n!}{(n+\alpha+\beta+1)_n} P_n^{\alpha,\beta}(x).$$

Hence,

$$P_n^{\alpha,\beta}(x) = \sum_{k=0}^{n} \binom{n}{k} \frac{(n+\alpha+\beta+1)_k \Gamma(n+\alpha+1)}{n!\Gamma(k+\alpha+1)} \left(\frac{x-1}{2}\right)^k \tag{4}$$

or

$$P_n^{\alpha,\beta}(x) = (-1)^n \sum_{k=0}^{n} \binom{n}{k} \frac{(n+\alpha+\beta+1)_k \Gamma(n+\beta+1)}{n!\Gamma(k+\beta+1)} \left(\frac{x+1}{-2}\right)^k. \tag{5}$$

The Chebyshev polynomials of the first kind $T_n(x)$ and the second kind $U_n(x)$ are defined by:

$$T_n(x) = \frac{P_n^{-\frac{1}{2},-\frac{1}{2}}(x)}{P_n^{-\frac{1}{2},-\frac{1}{2}}(1)}, \quad \frac{U_n(x)}{n+1} = \frac{P_n^{\frac{1}{2},\frac{1}{2}}(x)}{P_n^{\frac{1}{2},\frac{1}{2}}(1)}. \tag{6}$$

Therefore, substituting into $T_n(x)$ and $U_n(x)$ of (6) respectively with (4) or (5), the Chebyshev expansions into power series of $(x+1)$ or $(1-x)$ are obtained. The Chebyshev polynomials of the first kind, for instance, can be expanded as

$$T_n(x) = \sum_{k=0}^{n} (-1)^n \binom{n}{k} \frac{(n)_k \Gamma(n+\frac{1}{2})}{(\frac{1}{2})_n \Gamma(k+\frac{1}{2})} \left(\frac{x+1}{-2}\right)^k,$$

or

$$T_n(x) = \sum_{k=0}^{n} (-1)^k \binom{n}{k} \frac{(n)_k \Gamma(n+\frac{1}{2})}{(\frac{1}{2})_n \Gamma(k+\frac{1}{2})} \left(\frac{1-x}{2}\right)^k.$$

Now, we derive the direct formulae for computing the fractional derivatives. Let us denote ${}_{-1}^{C}D_x^{\gamma}$ and ${}_{-1}^{RL}D_x^{\gamma}$ the left Caputo fractional derivatives and left Riemann-Liouville fractional derivatives with $n-1 \le \gamma < n$, respectively, that is (see [25]),

$$\begin{aligned} {}_{-1}^{C}D_x^{\gamma} u(x) &= \frac{1}{\Gamma(n-\gamma)} \int_{-1}^{x} \frac{u^{(n)}(s)ds}{(x-s)^{-n+\gamma+1}}, \\ {}_{-1}^{RL}D_x^{\gamma} u(x) &= \frac{1}{\Gamma(n-\gamma)} \frac{d^n}{dx^n} \int_{-1}^{x} \frac{u(s)ds}{(x-s)^{-n+\gamma+1}}. \end{aligned}$$

Similarly, denote the right Caputo fractional derivatives and right Riemann-Liouville fractional derivatives by ${}_{x}^{C}D_1^{\gamma}$ and ${}_{x}^{RL}D_1^{\gamma}$ for $n-1 \le \gamma < n$, respectively, which are defined as

$$\begin{aligned} {}_{x}^{C}D_1^{\gamma} u(x) &= \frac{(-1)^n}{\Gamma(n-\gamma)} \int_{x}^{1} \frac{u^{(n)}(s)ds}{(s-x)^{-n+\gamma+1}}, \\ {}_{x}^{RL}D_1^{\gamma} u(x) &= \frac{(-1)^n}{\Gamma(n-\gamma)} \frac{d^n}{dx^n} \int_{x}^{1} \frac{u(s)ds}{(s-x)^{-n+\gamma+1}}. \end{aligned}$$

The integrals above exist almost everywhere for $u \in AC^n[-1,1]$.

Here, we mainly consider the computation of fractional derivatives of order $0 < \gamma < 2$. Let us keep the following relations in mind

$$ {}_{-1}^{C}D_x^{\alpha}u(x) = {}_{-1}^{RL}D_x^{\alpha}\left[u(x) - \sum_{k=0}^{n-1}\frac{u^{(k)}(-1)}{k!}(x+1)^k\right], \tag{7} $$

$$ {}_{x}^{C}D_1^{\alpha}u(x) = {}_{x}^{RL}D_1^{\alpha}\left[u(x) - \sum_{k=0}^{n-1}(-1)^k\frac{u^{(k)}(1)}{k!}(1-x)^k\right] \tag{8} $$

for any $n-1 \le \alpha < n$.

By (6) and combining with (4),(5), we can directly obtain the following formulae

$$ {}_{-1}^{RL}D_x^{\gamma}T_m(x) = \sum_{j=0}^{m}(-1)^{m-j}\binom{m}{j}\frac{(m)_j\Gamma(j+1)}{2^j(\frac{1}{2})_j\Gamma(j-\gamma+1)}(x+1)^{j-\gamma}, \tag{9} $$

$$ {}_{x}^{RL}D_1^{\gamma}T_m(x) = \sum_{j=0}^{m}(-1)^{j}\binom{m}{j}\frac{(m)_j\Gamma(j+1)}{2^j(\frac{1}{2})_j\Gamma(j-\gamma+1)}(1-x)^{j-\gamma}, \tag{10} $$

since

$$ {}_{-1}^{RL}D_x^{\gamma}[(x+1)^{\beta}] = \frac{\Gamma(\beta+1)}{\Gamma(\beta-\gamma+1)}(x+1)^{\beta-\gamma},\ {}_{x}^{RL}D_1^{\gamma}[(1-x)^{\beta}] = \frac{\Gamma(\beta+1)}{\Gamma(\beta-\gamma+1)}(1-x)^{\beta-\gamma} $$

for any $\beta \in \mathbb{R}$. Note that

$$ T_m^{(k)}(-1) = \begin{cases} 0, & k > m, \\ (-1)^{m-k}\binom{m}{k}\dfrac{(m)_k\Gamma(k+1)}{2^k(\frac{1}{2})_k}, & k \le m. \end{cases} $$

Thus,

$$ T_m(x) - \sum_{k=0}^{n-1}\frac{T_m^{(k)}(-1)}{k!}(x+1)^k = \begin{cases} 0, & 0 \le m \le n-1, \\ \displaystyle\sum_{j=n}^{m}(-1)^{m-j}\binom{m}{j}\frac{(m)_j}{2^j(\frac{1}{2})_j}(x+1)^j, & m \ge n. \end{cases} $$

Substituting the last identity into (7) and employing (9), then we can obtain the Caputo fractional derivatives as

$$ {}_{-1}^{C}D_x^{\gamma}T_m(x) = \sum_{j=\mathrm{Id}(\gamma)}^{m}(-1)^{m-j}\binom{m}{j}\frac{(m)_j\Gamma(j+1)}{2^j(\frac{1}{2})_j\Gamma(j-\gamma+1)}(x+1)^{j-\gamma} \tag{11} $$

for $m \ge \mathrm{Id}(\gamma)$, where

$$ \mathrm{Id}(\gamma) = \begin{cases} 1, & 0 < \gamma < 1, \\ 2, & 1 < \gamma < 2, \end{cases} $$

and ${}_{-1}^{C}D_x^{\gamma}T_m(x) = 0$ for other m's. Similarly,

$$ {}_{x}^{C}D_1^{\gamma}T_m(x) = \sum_{j=\mathrm{Id}(\gamma)}^{m}(-1)^{j}\binom{m}{j}\frac{(m)_j\Gamma(j+1)}{2^j(\frac{1}{2})_j\Gamma(j-\gamma+1)}(1-x)^{j-\gamma} \tag{12} $$

for $m \ge \mathrm{Id}(\gamma)$, and ${}_{x}^{C}D_1^{\gamma}T_m(x) = 0$ for other m's.

Thereafter, we designate the formulas (9)-(12) as Method-I.

3. Recurrence formulae for fractional derivatives

In this section, we shall make use of the properties of the Chebyshev polynomials of the second kind to gain the recurrence algorithms for computations of the left and right Caputo and Riemann-Liouville fractional derivatives.

The Chebyshev polynomials of the second kind $U_n(x)$ may be explicitly written as

$$U_n(x) = \frac{\sin[(n+1)\arccos x]}{\sqrt{1-x^2}},\ n = 0, 1, 2, \cdots.$$

Especially,

$$T'_{n+1}(x) = (n+1)U_n(x), \quad T''_{n+1}(x) = (n+1)U'_n(x),$$

and the corresponding three-term recurrence relation of the Chebyshev polynomials of the second kind is

$$\begin{cases} U_0(x) = 1, \quad U_1(x) = 2x, \\ U_{n+1}(x) = 2xU_n(x) - U_{n-1}(x),\ n \geq 1. \end{cases}$$

The following two properties are needed in the present paper.

Proposition 3.1 ([28]). *For $T_n(x)$ and $U_n(x)(n = 2, 3, \cdots)$, the following relation holds:*

$$2T_n(x) = U_n(x) - U_{n-2}(x), \tag{13}$$

and $U_n(-1) = (-1)^n n, U_n(1) = n$ for $n = 0, , 1, 2, \cdots$.

Proposition 3.2 ([28]). *The Chebyshev polynomials of the second kind satisfy the following formula*

$$2U_n(x) = \frac{U'_{n+1}(x)}{n+1} - \frac{U'_{n-1}(x)}{n+1}.$$

Now, we firstly compute the left Caputo fractional derivatives of γ order with $0 < \gamma < 1$ by two steps. Let ${}^L D_m^\gamma(x) = {}_{-1}^{C}D_x^\gamma T_m(x)$.

Step 1. Compute the fractional integral of $U_m(x)$. We denote $B_m^\alpha(x) = \frac{1}{\Gamma(\alpha)}\int_{-1}^{x}(x-s)^{\alpha-1}U_m(s)ds$ with $\alpha > 0$. Then, it is easy to obtain

$$B_0^\alpha(x) = \frac{(x+1)^\alpha}{\Gamma(1+\alpha)}, \quad B_1^\alpha(x) = \frac{2(x+1)^{1+\alpha}}{\Gamma(2+\alpha)} - \frac{2(x+1)^\alpha}{\Gamma(1+\alpha)}.$$

By using the recurrence relation, we have

$$\begin{aligned} B_{n+1}^\alpha(x) &= \frac{1}{\Gamma(\alpha)}\int_{-1}^{x}(x-s)^{\alpha-1}U_{n+1}(s)ds \\ &= \frac{1}{\Gamma(\alpha)}\int_{-1}^{x}(x-s)^{\alpha-1}[2sU_n(s) - U_{n-1}(s)]ds \\ &= 2xB_n^\alpha(x) - B_{n-1}^\alpha(x) - \frac{2}{\Gamma(\alpha)}\int_{-1}^{x}(x-s)^\alpha U_n(s)ds. \end{aligned}$$

By Proposition 3.2,

$$\begin{aligned} B_{n+1}^\alpha(x) =& 2xB_n^\alpha(x) - B_{n-1}^\alpha(x) \\ &- \frac{1}{(n+1)\Gamma(\alpha)}\int_{-1}^{x}(x-s)^\alpha\left[U'_{n+1}(x) - U'_{n-1}(s)\right]ds \\ =& 2xB_n^\alpha(x) - B_{n-1}^\alpha(x) - \frac{\alpha B_{n+1}^\alpha(x)}{n+1} + \frac{\alpha B_{n-1}^\alpha(x)}{(n+1)} - \frac{(-1)^n \cdot 2(x+1)^\alpha}{(n+1)\Gamma(\alpha)}. \end{aligned}$$

By rearrangement, we have

$$B_{n+1}^{\alpha}(x) = \frac{2x(n+1)}{n+1-\alpha}B_n^{\alpha}(x) - \frac{n+1-\alpha}{n+1+\alpha}B_{n-1}^{\alpha}(x) - \frac{(-1)^n \cdot 2(x+1)^{\alpha}}{(n+1+\alpha)\Gamma(\alpha)}.$$

Therefore, we can obtain the recurrence relation to compute $B_n^{\alpha}(x)$

(14)

$$\begin{cases} B_0^{\alpha}(x) = \dfrac{(x+1)^{\alpha}}{\Gamma(1+\alpha)}, \\ B_1^{\alpha}(x) = \dfrac{2(x+1)^{1+\alpha}}{\Gamma(2+\alpha)} - \dfrac{2(x+1)^{\alpha}}{\Gamma(1+\alpha)}, \\ B_{n+1}^{\alpha}(x) = \dfrac{2(n+1)x}{n+1+\alpha}B_n^{\alpha}(x) - \dfrac{(n+1-\alpha)}{n+1+\alpha}B_{n-1}^{\alpha}(x) - \dfrac{2(-1)^n(x+1)^{\alpha}}{(n+1+\alpha)\Gamma(\alpha)}, n \geq 1. \end{cases}$$

Step 2. Compute the left Caputo fractional derivatives ${}^{L}D_m^{\gamma}(x)$. Clearly,

$${}^{L}D_0^{\gamma}(x) = {}_{-1}^{C}D_x^{\gamma}T_0(x) = 0,\ {}^{L}D_1^{\gamma}(x) = {}_{-1}^{C}D_x^{\gamma}T_1(x) = \frac{(x+1)^{1-\gamma}}{\Gamma(2-\gamma)}.$$

By the second identity of (13), we derive for any $m \geq 1$ that

$$\begin{aligned} {}^{L}D_{m+1}^{\gamma}(x) &= \frac{1}{\Gamma(1-\gamma)}\int_{-1}^{x}(x-s)^{-\gamma}T'_{m+1}(s)ds \\ &= \frac{m+1}{\Gamma(1-\gamma)}\int_{-1}^{x}(x-s)^{-\gamma}U_m(s)ds = (m+1)B_m^{1-\gamma}(x). \end{aligned} \tag{15}$$

Therefore, the computation scheme of ${}^{L}D_m^{\gamma}(x) = {}_{-1}^{C}D_x^{\gamma}T_m(x) (0 < \gamma < 1)$ is as follows

$$\begin{cases} {}^{L}D_0^{\gamma}(x) = 0, \\ {}^{L}D_{m+1}^{\gamma}(x) = (m+1)B_m^{1-\gamma}(x), \text{ for } m \geq 0, \end{cases} \tag{16}$$

where $B_m^{1-\gamma}(x)$ is defined as (14). □

Secondly, we calculate the left Caputo fractional derivatives of $1+\gamma$ order with $0 < \gamma < 1$ by two steps. Let ${}^{L}D_m^{1+\gamma}(x) = {}_{-1}^{C}D_x^{1+\gamma}T_m(x)$.

Step 1. Compute the fractional integral of $U'_m(x)$. Note that $T''_n(x) = nU'_{n-1}(x)$, then it is sufficient to compute the fractional integral of $U'_n(x)$. Denote by $\hat{B}_m^{\alpha}(x) = \frac{1}{\Gamma(\alpha)}\int_{-1}^{x}(x-s)^{\alpha-1}U'_m(s)ds$. We have

$$\hat{B}_0^{\alpha}(x) = 0,\ \hat{B}_1^{\alpha}(x) = \frac{2(x+1)^{\alpha}}{\Gamma(1+\alpha)}. \tag{17}$$

Since $U'_{m+1}(x) = 2(m+1)U_m(x) + U'_{m-1}(x)$ by Proposition 3.2, thus for any $\alpha > 0$ and $m \geq 1$,

$$\begin{aligned} \hat{B}_{m+1}^{\alpha}(x) &= \frac{1}{\Gamma(\alpha)}\int_{-1}^{x}(x-s)^{\alpha-1}U'_{m+1}(s)ds \\ &= \frac{1}{\Gamma(\alpha)}\int_{-1}^{x}(x-s)^{\alpha-1}[2(m+1)U_m(s) + U'_{m-1}(s)]ds \\ &= 2(m+1)B_m^{\alpha}(x) + \hat{B}_{m-1}^{\alpha}(x). \end{aligned} \tag{18}$$

Step 2. Compute the left Caputo fractional derivatives ${}^{L}D_m^{1+\gamma}(x)$. For $m = 0, 1$,

$${}^{L}D_m^{1+\gamma}(x) = \frac{1}{\Gamma(1-\gamma)}\int_{-1}^{x}(x-s)^{-\gamma}T''_m(s)ds = 0.$$

For any $m \geq 2$, one can get

$$\begin{aligned} {}^{L}D_m^{1+\gamma}(x) &= \frac{1}{\Gamma(1-\gamma)} \int_{-1}^{x} (x-s)^{-\gamma} T_m''(s) ds \\ &= \frac{m}{\Gamma(1-\gamma)} \int_{-1}^{x} (x-s)^{-\gamma} U_{m-1}'(s) ds = m\hat{B}_{m-1}^{1-\gamma}(x). \end{aligned} \tag{19}$$

Therefore, we obtain the computation scheme of ${}^{L}D_m^{1+\gamma}(x) = {}_{-1}^{C}D_x^{1+\gamma} T_m(x)$ as follows

$$\begin{cases} {}^{L}D_0^{1+\gamma}(x) = {}^{L}D_1^{1+\gamma}(x) = 0, \\ {}^{L}D_m^{1+\gamma}(x) = m\hat{B}_{m-1}^{1-\gamma}(x),\ m \geq 2, \end{cases} \tag{20}$$

where $\hat{B}_m^{1-\gamma}(x)$ is defined in (17)-(18). □

Finally, we consider the computation of right fractional derivatives of order γ and $1+\gamma$ with $0 < \gamma < 1$. Similar to the process above, let

$$C_n^{\alpha}(x) = \frac{1}{\Gamma(\alpha)} \int_{x}^{1} (s-x)^{\alpha-1} U_n(s) ds$$

for $\alpha > 0$. Then, by some computations we have

(21)

$$\begin{cases} C_0^{\alpha}(x) = \dfrac{(1-x)^{\alpha}}{\Gamma(1+\alpha)}, \\ C_1^{\alpha}(x) = -\dfrac{2(1-x)^{1+\alpha}}{\Gamma(2+\alpha)} + \dfrac{2(1-x)^{\alpha}}{\Gamma(1+\alpha)}, \\ C_{n+1}^{\alpha}(x) = \dfrac{2(n+1)x}{n+1+\alpha} C_n^{\alpha}(x) - \dfrac{n+1-\alpha}{n+1+\alpha} C_{n-1}^{\alpha}(x) + \dfrac{2(1-x)^{\alpha}}{(n+1+\alpha)\Gamma(\alpha)}, n \geq 1. \end{cases}$$

Denote $\hat{C}_n^{\alpha}(x) = \frac{1}{\Gamma(\alpha)} \int_x^1 (s-x)^{\alpha-1} U_n'(s) ds$. Then it can be obtained that

$$\begin{cases} \hat{C}_0^{\alpha}(x) = 0,\ \hat{C}_1^{\alpha}(x) = \dfrac{2(1-x)^{\alpha}}{\Gamma(1+\alpha)}, \\ \hat{C}_{n+1}^{\alpha}(x) = 2(n+1) C_n^{\alpha}(x) + \hat{C}_{n-1}^{\alpha}(x),\ n \geq 1. \end{cases} \tag{22}$$

Denote ${}^{R}D_m^{\gamma}(x) = {}_{x}^{C}D_1^{\gamma} T_m(x)$, ${}^{R}D_m^{1+\gamma}(x) = {}_{x}^{C}D_1^{1+\gamma} T_m(x)$ for $0 < \gamma < 1$. Then, similar to (15) and (20) we can derive

$$\begin{cases} {}^{R}D_0^{\gamma}(x) = 0, \\ {}^{R}D_m^{\gamma}(x) = -mC_{m-1}^{1-\gamma}(x),\ m \geq 1, \end{cases} \tag{23}$$

and

$$\begin{cases} {}^{R}D_0^{1+\gamma}(x) = {}^{R}D_1^{1+\gamma}(x) = 0, \\ {}^{R}D_m^{1+\gamma}(x) = m\hat{C}_{m-1}^{1-\gamma}(x),\ m \geq 2. \end{cases} \tag{24}$$

Hereafter, we designate this recurrence algorithm as Method-II.

4. Fractional differentiation matrices and consistency analysis

4.1. Left and right fractional differentiation matrices. Denote by $\{\hat{x}_j\}_{j=0}^{N}$ the collocation points on $[-1, 1]$. Let $l_j(x)$ be the Lagrange interpolation functions based on $\hat{x}_j$ for $j = 0, 1, 2, \cdots, N$,

$$l_j(x) = \prod_{\substack{k=0 \\ k \neq j}}^{N} \frac{x - \hat{x}_k}{\hat{x}_j - \hat{x}_k}.$$

Here, we make use of the Gauss-Chebyshev-Lobatto points as the collocation points.

Let

$$D_\gamma^L = (D_{ij}^L)_{M\times(N+1)},\ D_{ij}^L = {}_{-1}^{RL}D_x^\gamma l_j(x_i), \tag{25}$$

$$D_\gamma^R = (D_{ij}^R)_{M\times(N+1)},\ D_{ij}^R = {}_{x}^{RL}D_1^\gamma l_j(x_i). \tag{26}$$

where $x_1, x_2, \cdots, x_M$ are grid points. The matrices D_γ^L, D_γ^R are called the left and right fractional differentiation matrices. In the following, we shall establish these matrices. To the end, we first expand $l_j(x)$ by using the Chebyshev polynomials

$$l_j(x) = \sum_{k=0}^{N} b_k^j T_k(x),$$

where

$$b_k^j = \begin{cases} \frac{1}{\pi}(l_j(x), T_k(x))_{w^{-1/2,-1/2}},\ k = 0, \\ \frac{2}{\pi}(l_j(x), T_k(x))_{w^{-1/2,-1/2}},\ k = 1, 2, \cdots. \end{cases}$$

Therefore, the k^{th} column of the differentiation matrix is derived by

$$D_{\cdot k}^L = {}_{-1}^{RL}D_x^\gamma l_k(\cdot) = \sum_{j=0}^{N} b_j^k \cdot {}_{-1}^{RL}D_x^\gamma T_j(\cdot)$$

or

$$D_{\cdot k}^R = {}_{x}^{RL}D_1^\gamma l_k(\cdot) = \sum_{j=0}^{N} b_j^k \cdot {}_{x}^{RL}D_1^\gamma T_j(\cdot)$$

for $k = 0, 1, \cdots, N$.

Consider a uniform grid $\{x_1, x_2, \cdots, x_M\}$ and a set of data $\{u_0, u_1, \cdots, u_N\}$ obtained from a certain suitably regular function $u(x)$ at the collocation points, then the discrete left fractional derivatives ${}_{-1}^{RL}D_x^\gamma u(x_j)$ are obtained by

$$\begin{pmatrix} {}_{-1}^{RL}D_x^\gamma u(x_1) \\ {}_{-1}^{RL}D_x^\gamma u(x_2) \\ \cdots \\ {}_{-1}^{RL}D_x^\gamma u(x_M) \end{pmatrix} = D_\gamma^L \cdot U = \begin{bmatrix} D_{10}^L & D_{11}^L \cdots & D_{1N}^L \\ D_{20}^L & D_{21}^L \cdots & D_{2N}^L \\ \cdots & \cdots\cdots & \cdots \\ D_{M0}^L & D_{M1}^L \cdots & D_{MN}^L \end{bmatrix} \begin{pmatrix} u_0 \\ u_1 \\ \cdots \\ u_N \end{pmatrix}.$$

Analogically, the discrete right fractional derivatives can be obtained by right fractional differentiation matrix, that is, by $D_\gamma^R \cdot U$.

By using Method-I and Method-II, two types of schemes to compute the differentiation matrices can be obtained. However, Method-I may cause instability with N increasing. In what follows, we shall compare the performance of recurrence algorithm to that of direct method.

Example 1. Consider the computation of left fractional derivatives of polynomial function $u(x) = (1 - x^2)^2$.

The maximum errors of the left Riemann-Liouville fractional derivatives of function $u(x)$ are obtained by using different schemes, Method-I and Method-II, respectively. The results are shown in Figure 1, where two orders of fractional derivative $0 < \gamma < 1$ are considered. From the plots we see that the maximum errors by Method-I are increasing when the polynomial degree $N > 20$, and the approximation getd worse as $N > 30$ and faild to converge even, whereas the results by Method-II are very satisfactory.

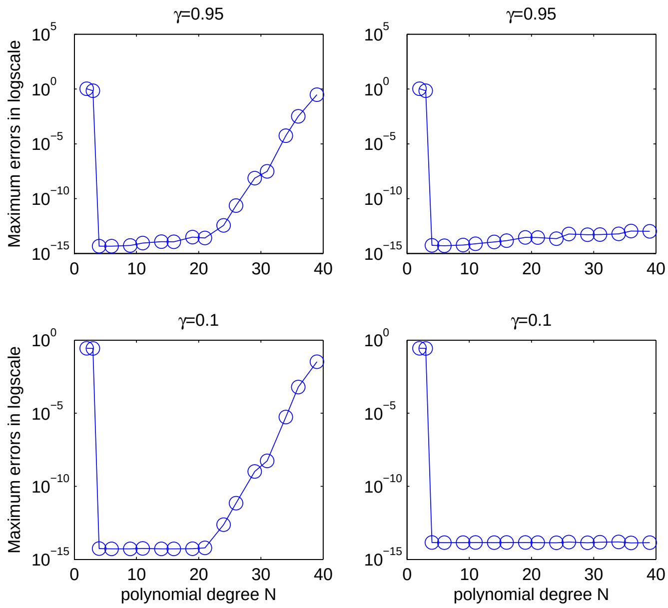

FIGURE 1. The left Riemann-Liouville fractional derivatives of $(1-x^2)^2$. Left column: the maximum errors by Method-I. Right column: the maximum errors by Method-II.

Example 2. Consider the left Riemann-Liouville fractional derivatives of a finite regular function $u(x) = (x+1)^{\frac{9}{2}}$.

Here, we consider the order $\gamma = 0.9$. The results are shown in Figure 2 which are plotted in log-log scale. Figure 2 illustrates Method-I is stable for $N \leq 20$, and both methods have the same accuracy, whereas in case of $N > 20$ only Method-II is still effective. It can also be seen that only the accuracy of 1E-08 is attained by Method-I. Figure 2 shows also that an algebraic convergence is obtained for the finite regular problem by Method-II.

Example 3. Consider the left Riemann-Liouville fractional derivatives of function $u(x) = e^x$ for order $0 < \gamma < 1$.

In this example we compute the left fractional derivatives of a smooth and infinitely differentiable function as order $\gamma \in (0, 1)$. The results are shown in Figure 3 which are plotted in log scale. It can be seen that both methods are exponentially convergent from Figure 3, which converge to the computer precision fast. However, Method-I is unstable when $N > 23$.

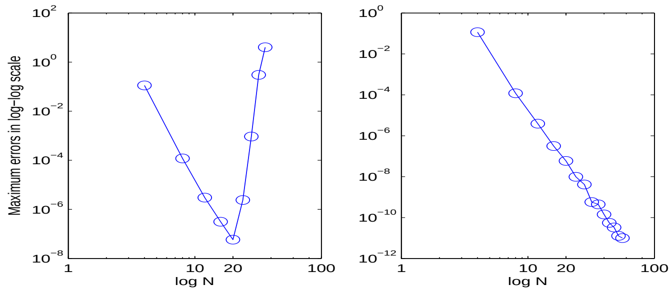

FIGURE 2. The left Riemann-Liouville fractional derivatives of $(x+1)^{\frac{9}{2}}$ with order $\gamma = 0.9$. Left: the maximum errors by Method-I. Right: the maximum errors by Method-II.

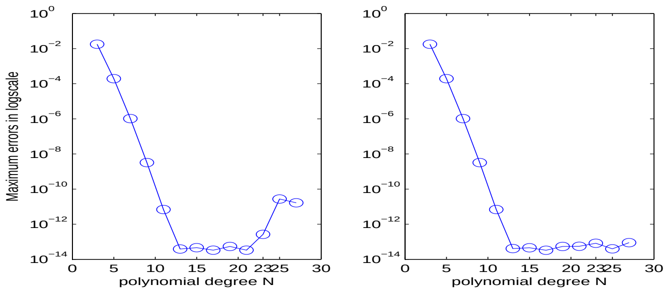

FIGURE 3. The left Riemann-Liouville fractional derivatives of e^x with order $\gamma = 0.5$. Left: the maximum errors by Method-I. Right: the maximum errors by Method-II.

Example 4. Consider the right Riemann-Liouville fractional derivatives of function $u(x) = e^x$ for order $1 < \gamma < 2$.

In this example we compute the right fractional derivatives of a smooth and infinitely differentiable function as order $\gamma = 1.9, 1.1$. The results are shown in Figure 4 which are plotted in log scale. It can be also seen that both methods are exponentially convergent from Figure 4, which converge to the computer precision 1E-14 fast. However, Method-I is unstable when $N > 20$.

4.2. Consistency error analysis. Set $\Lambda = (-1, 1)$, and $w^{\alpha,\beta}(x) = (1-x)^\alpha(1+x)^\beta$. Denote by $(\cdot,\cdot)$ and $(\cdot,\cdot)_{w^{\alpha,\beta}}$ the inner products of the Hilbert spaces $L^2(\Lambda)$ and $L^2_{w^{\alpha,\beta}}(\Lambda)$, by $\|\cdot\|$ the L^2- norm and $\|\cdot\|_{w^{\alpha,\beta}}$ the weighted L^2-norm. Let $H^m_{w^{\alpha,\beta},*}(\Lambda)$ be the non-uniformly Jacobi-weighted Sobolev space [9]:

$$H^m_{w^{\alpha,\beta},*}(\Lambda) = \{v|v \text{ is measurable and } \|v\|_{m,w^{\alpha,\beta},*} < \infty\},\ m \in \mathbb{N},$$

equipped with the following norm and semi-norm,

$$\|v\|_{m,w^{\alpha,\beta},*} = \left(\sum_{k=0}^{m} \|\partial_x^k v\|^2_{w^{\alpha+k,\beta+k}}\right)^{1/2},\ |v|_{m,w^{\alpha,\beta},*} = \|\partial_x^m v\|_{w^{\alpha+m,\beta+m}}.$$

Denote by $I_N u$ the Lagrange interpolation of u. Note that ${}^{RL}_{-1}D^\gamma_x I_N u = D^L_\gamma \cdot U$, and ${}^{RL}_{x}D^\gamma_1 I_N u = D^R_\gamma \cdot U$. Then, we have the following error estimation for

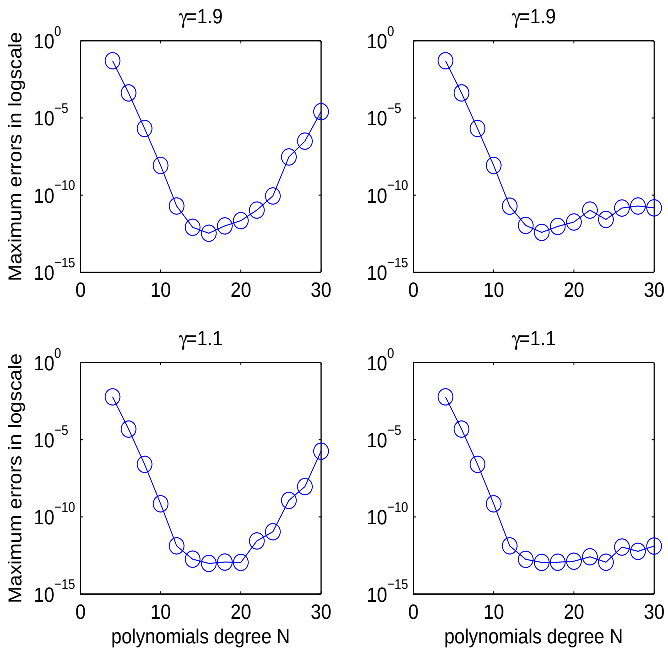

FIGURE 4. The right Riemann-Liouville fractional derivatives of e^x with order γ. Left: the maximum errors by Method-I. Right: the maximum errors by Method-II.

interpolation, which is also used to illustrate high order accuracy of the spectral collocation method.

Theorem 4.1. *Let $u \in H^m_{w^{-1/2,-1/2},*}(\Lambda)$ with $m > \gamma$. Then, we have*

$$\|{}^{RL}_{-1}D^\gamma_x(u - I_N u)\|_{w^{-1/2,-1/2+2\gamma}} \le CN^{\gamma-m}\|\partial^m_x u\|_{w^{-1/2+m,-1/2+m}}, \tag{27}$$

$$\|{}^{RL}_{x}D^\gamma_1(u - I_N u)\|_{w^{-1/2+2\gamma,-1/2}} \le CN^{\gamma-m}\|\partial^m_x u\|_{w^{-1/2+m,-1/2+m}}, \tag{28}$$

where C is a constant independent of N and u.

Proof The proof of this theorem is provided in Appendix. □

5. Applications to fractional differential equations

In this section, we shall solve some linear and nonlinear fractional differential equations by spectral collocation method based on the recurrence algorithm, Method-II, to demonstrate the performance of our new method. Hereafter, we take the Gauss-Chebyshev-Lobatto nodes as the collocation points.

5.1. General fractional derivatives. At first, we consider the computations of the general fractional derivatives ${}^{RL}_aD^\gamma_x u(x)$, ${}^{RL}_xD^\gamma_b u(x)$, ${}^{RL}_aD^{1+\gamma}_x u(x)$, and ${}^{RL}_xD^{1+\gamma}_b u(x)$ for $\gamma \in (0, 1)$ and $x \in [a, b]$.

Let $x = \frac{a+b}{2} + \frac{b-a}{2}\xi$ $(-1 \le \xi \le 1)$, and denote $\hat{u}(\xi) = u(\frac{a+b}{2} + \frac{b-a}{2}\xi)$. Notice that

$$u'(x) = \frac{2}{b-a}\hat{u}'(\xi),\ u''(x) = \left(\frac{2}{b-a}\right)^2 \hat{u}''(\xi).$$

Thus, for general left fractional derivatives one has

$$ {}_a^C D_x^\gamma u(x) = \frac{1}{\Gamma(1-\gamma)} \int_a^x (x-s)^{-\gamma} \frac{\partial u}{\partial s}(s) ds = \left(\frac{b-a}{2}\right)^{-\gamma} {}_{-1}^C D_\xi^\gamma \hat{u}(\xi), \tag{29} $$

and,

$$ {}_a^C D_x^{1+\gamma} u(x) = \frac{1}{\Gamma(1-\gamma)} \int_a^x (x-s)^{-\gamma} \frac{\partial^2 u}{\partial s^2}(s) ds = \left(\frac{b-a}{2}\right)^{-1-\gamma} {}_{-1}^C D_\xi^{1+\gamma} \hat{u}(\xi). \tag{30} $$

For general right fractional derivatives,

$$ {}_x^C D_b^\gamma u(x) = \frac{-1}{\Gamma(1-\gamma)} \int_x^b (s-x)^{-\gamma} \frac{\partial u}{\partial s}(s) ds = \left(\frac{b-a}{2}\right)^{-\gamma} {}_\xi^C D_1^\gamma \hat{u}(\xi), \tag{31} $$

$$ {}_x^C D_b^{1+\gamma} u(x) = \frac{1}{\Gamma(1-\gamma)} \int_x^b (s-x)^{-\gamma} \frac{\partial^2 u}{\partial s^2}(s) ds = \left(\frac{b-a}{2}\right)^{-1-\gamma} {}_\xi^C D_1^{1+\gamma} \hat{u}(\xi). \tag{32} $$

Hence, the Riemann-Liouville fractional derivatives are obtained as

$$ \begin{aligned} {}_a^{RL} D_x^\gamma u(x) &= {}_a^C D_x^\gamma u(x) + \frac{u(a)}{\Gamma(1-\gamma)}(x-a)^{-\gamma} \\ &= \left(\frac{b-a}{2}\right)^{-\gamma} \left[{}_{-1}^C D_\xi^\gamma \hat{u}(\xi) + \frac{\hat{u}(-1)}{\Gamma(1-\gamma)}(\xi+1)^{-\gamma} \right], \end{aligned} \tag{33} $$

and

$$ \begin{aligned} {}_a^{RL} D_x^{1+\gamma} u(x) &= {}_a^C D_x^{1+\gamma} u(x) + \frac{u'(a)}{\Gamma(1-\gamma)}(x-a)^{-\gamma} + \frac{u(a)}{\Gamma(-\gamma)}(x-a)^{-1-\gamma} \\ &= \left(\frac{b-a}{2}\right)^{-1-\gamma} \left[{}_{-1}^C D_\xi^{1+\gamma} \hat{u}(\xi) + \frac{\hat{u}(-1)}{\Gamma(1-\gamma)}(\xi+1)^{-\gamma} + \frac{\hat{u}(-1)}{\Gamma(-\gamma)}(\xi+1)^{-1-\gamma} \right]. \end{aligned} \tag{34} $$

Similarly,

$$ {}_x^{RL} D_b^\gamma u(x) = \left(\frac{b-a}{2}\right)^{-\gamma} \left[{}_\xi^C D_1^\gamma \hat{u}(\xi) + \frac{\hat{u}(1)}{\Gamma(1-\gamma)}(1-\xi)^{-\gamma} \right], \tag{35} $$

$$ \begin{aligned} {}_x^{RL} D_b^{1+\gamma} u(x) = \left(\frac{b-a}{2}\right)^{-1-\gamma} &\left[{}_\xi^C D_1^{1+\gamma} \hat{u}(\xi) - \frac{\hat{u}(1)}{\Gamma(1-\gamma)}(1-\xi)^{-\gamma} \right. \\ &\left. + \frac{\hat{u}(1)}{\Gamma(-\gamma)}(1-\xi)^{-1-\gamma} \right]. \end{aligned} \tag{36} $$

5.2. Multi-term fractional differential equations. The spectral collocation method can be applied to solve various multi-term fractional differential equations effectively. Here, we only consider a two-term steady-state linear fractional equation

$$ \begin{cases} d_1 {}_{-1}^{RL} D_x^{r_1} u(x) + d_2 {}_{-1}^{RL} D_x^{1+r_2} u(x) = f(x), \; x \in (-1,1) \\ u(-1) = 0, u(1) = u_r = 2^{6+9/17}, \end{cases} \tag{37} $$

where $0 < r_1, r_2 < 1$, d_1, d_2 are constants and

$$ f(x) = \frac{\Gamma(\frac{128}{17})}{\Gamma(\frac{128}{17} - r_1)}(1+x)^{\frac{111}{17} - r_1} - \left(\frac{111}{17} - r_2\right) \frac{\Gamma(\frac{128}{17})}{\Gamma(\frac{128}{17} - r_2)}(1+x)^{\frac{94}{17} - r_2}. $$

We take $d_1 = 1, d_2 = -1$. This problem (37) comes from [33] whose exact solution is $u(x) = (1+x)^{6+9/17}$. Here, the exact solution has finite regularity like $H^7(\Lambda)$. Let $P_N(\Lambda)$ be the set of polynomials of degree at most N. Let $x_j (j =$

$0, 1, 2, \cdots, N)$ be the collocation points. The spectral collocation method for solving (37) is to find solution $u_N(x) \in P_N(\Lambda)$ such that

$$
{}_{-1}^{RL}D_x^{r_1} u_N(x)|_{x_j} - {}_{-1}^{RL}D_x^{1+r_2} u_N(x)|_{x_j} = f(x_j),\ j = 1, 2, \cdots, N-1. \tag{38}
$$

Let $u_N(x) = \sum_{j=0}^{N} u_N(x_j) l_j(x)$, where $l_j(x)$ are the Lagrange interpolation functions based on nodes $x_j (j = 0, 1, \cdots, N)$. Substituting $u_N(x)$ into (38), a system of equations is obtained:

$$
(D_{r_1}^L - D_{1+r_2}^L) U = F, \tag{39}
$$

where $U = (U_0, U_1, \cdots, U_N)^T$ with $U_k \approx u_N(x_k)$, $F = (f(x_1), f(x_2), \cdots, f(x_{N-1}))^T$. Considering the boundary conditions, it gives that $U_0 = u_N(x_0) = 0, U_N = u_N(x_N) = u_r$. Adding these two equations to (39) a closed linear system is derived.

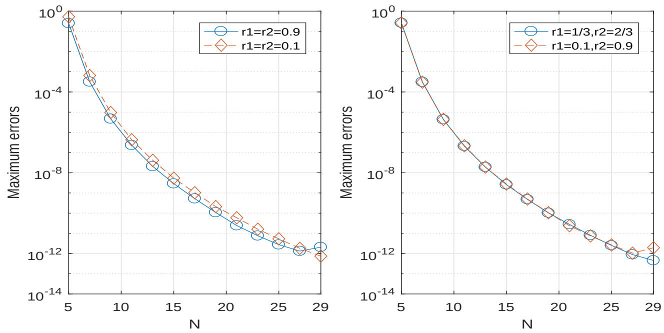

FIGURE 5. Multi-term fractional differential equation: the maximum errors of (37) in log-scale, versus N.

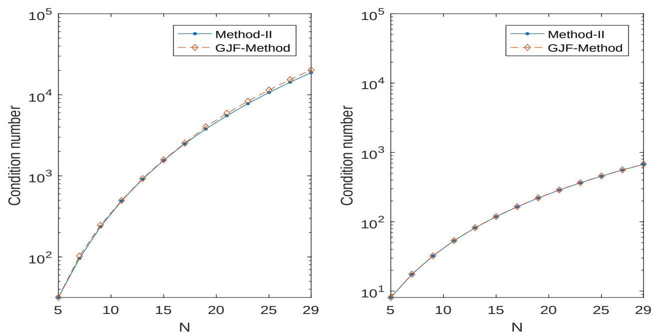

FIGURE 6. Multi-term fractional differential equation (37): the comparison of corresponding condition numbers corresponding to GJF-Method and Method-II, in log-scale versus N, for $r_1 = 1/3$, $r_2 = 2/3$ (Left), and $r_1 = r_2 = 0.1$ (Right).

Here, we consider four cases: $r_1 = r_2 = 0.9$, $r_1 = r_2 = 0.1$, $r_1 = 1/3, r_2 = 2/3$, $r_1 = 0.1, r_2 = 0.9$. The maximum errors in log-scale versus N are plotted in Figure 5. It can be seen that the same convergence (algebraic convergence) is obtained for these four cases. In order to compare our method with that from [33], in Figure 6 we plot the corresponding condition number of the linear system resulting from fractional differentiation matrix in log-scale versus N. It indicates that our method (Method-II) works better than that from [33] (GJF-Method).

Figure 6 also tells us that the condition number of the linear system for solving (37) is dominated by the diffusion index r_2. The larger the index r_2 is, the larger the condition number becomes.

5.3. Time-dependent FPDEs. We examine time-dependent FPDEs where the temporal derivative is fractional derivative (Caputo- or Riemann-Liouville-type) and the spatial derivative is left or right Riemann-Liouville fractional derivative.

5.3.1. Time- and space-fractional advection-diffusion equations. We consider the following problem from [33]

(40)
$$\begin{cases} {}_{0}^{RL}D_t^{\tau}u(x,t) + c\,{}_{-1}^{RL}D_x^{r_1}u(x,t) - K\,{}_{-1}^{RL}D_x^{1+r_2}u(x,t) = f(x,t),\ x \in (-1,1), t \in (0,T], \\ u(x,0) = 0, u(-1,t) = 0, u(1,t) = u_r(t), \end{cases}$$

where $\tau, r_1, r_2 \in (0,1)$, and c, K are constants.

Let $t' = \frac{2}{T}t - 1$, $\hat{u}(x,t') = u\left(x,(1+t')T/2\right)$. By (33) and the initial condition of (40), the problem above is reformulated as

$$(T/2)^{-\tau}\,{}_{-1}^{RL}D_{t'}^{\tau}\hat{u}(x,t') + c\,{}_{-1}^{RL}D_x^{r_1}\hat{u}(x,t') - K\,{}_{-1}^{RL}D_x^{1+r_2}\hat{u}(x,t') = \hat{f}(x,t') \tag{41}$$

for $x \in (-1,1), t' \in (-1,1)$, and prescribed with initial-boundary conditions

$$\hat{u}(x,-1) = 0, \hat{u}(-1,t') = 0, u(1,t') = \hat{u}_r(t')$$

where $\hat{f}(x,t') = f(x, \frac{T}{2} + \frac{T}{2}t'), \hat{u}_r(t') = u_r(\frac{T}{2} + \frac{T}{2}t')$.

Set

$$W_L = \mathrm{Span}\{l_i^t(t')l_j^x(x), i = 0,1,\cdots,M, j = 0,1,\cdots,N\},$$

where $l_i^t(t')$ is the Lagrange polynomials of degree M and $l_j^x(x)$ the Lagrange polynomials of degree N based on the Gauss-Chebyshev-Lobatto nodes on [-1,1]. We find $u_L(x,t') \in W_L$ such that u_L satisfies the initial-boundary problem (41). Let $u_L(x,t') = \sum_{i=0}^{M}\sum_{j=0}^{N} u_{ij}l_i^t(t')l_j^x(x)$. The zero initial and boundary conditions yield that u_{0j} and u_{i0} are zero for $i = 0,1,2,\cdots,M$ and $j = 0,1,2,\cdots,N$. Then, making use of the other nodes the following linear system of equations is derived

$$\left[(T/2)^{-\tau}E_{N-1} \otimes D_{\tau}^L\right]U + \left[(cD_{r_1}^L - KD_{1+r_2}^L) \otimes E_M\right]U = F, \tag{42}$$

where E_{N-1} and E_M are identity matrices of order $N-1$ and M respectively, and $\otimes$ stands for Kronecker product.

$$U = [u_{11}, u_{21}, \cdots, u_{M1}, u_{12}, u_{22}, \cdots, u_{M2}, \cdots, u_{1,N}, u_{2,N}, \cdots, u_{M,N}]^T,$$
$$F = [f_{11}, f_{21}, \cdots, f_{M1}, f_{12}, f_{22}, \cdots, f_{M2}, \cdots, f_{1,N-1}, f_{2,N-1}, \cdots, f_{M,N-1}]^T$$

with $f_{ij} = \hat{f}(x_j, t'_i)$. The boundary conditions $u_L(x_N, t') = \hat{u}_r(t')$ are considered to complement the system of equations (42) as a close system. Noting that the coefficient matrix of (42) is a band matrix, many classical approaches for solving linear algebra systems can be used to obtain these unknowns u_{ij}.

In light of [33], for the exact solution $u(x,t) = t^{6+\frac{2}{3}}\left[(1+x)^{6+\frac{9}{17}} - 2(1+x)^{5+\frac{9}{17}}\right]$ we study the temporal accuracy of our method. Here, we consider the fractional advection-diffusion equations with $T = 1$, whose orders are $r_1 = 0.1, r_2 = 0.9$ and $r_1 = 1/3, r_2 = 2/3$ respectively. For both cases, the time fractional derivatives of order $\tau = 0.1$ and $\tau = 0.9$ are investigated. Numerical results at $t = 1$ are shown in Figure 7, where the left panel corresponds to the orders $r_1 = 0.1, r_2 = 0.9$, and the right panel to $r_1 = 1/3, r_2 = 2/3$. Clearly, they show that our method is exponentially convergent for the time discretization. Additionally, our method is also efficient for large degree M or N.

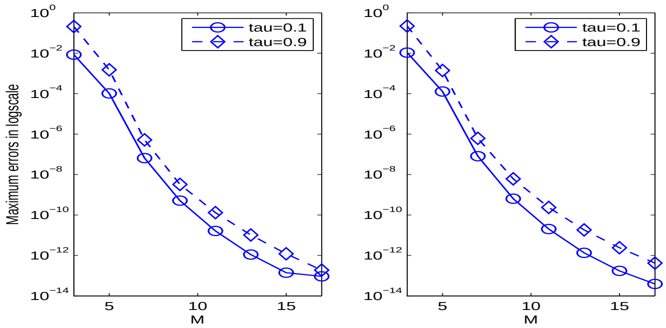

FIGURE 7. The maximum errors of (40) in log-scale, versus M with $N = 50$. Left: $r_1 = 0.1, r_2 = 0.9$; Right: $r_1 = 1/3, r_2 = 2/3$.

5.3.2. Time-space Riesz fractional diffusion equations. Especially, our method can be applied to solve the Riesz fractional PDEs.

Consider the following equation

$$\begin{cases} {}_0^C D_t^\alpha u(x,t) = \dfrac{\partial^{2\beta}}{\partial|x|^{2\beta}} u(x,t) + f(x,t), (x,t) \in (-1,1] \times (0,1], \\ u(x,0) = 0, x \in (-1,1), \\ u(-1,t) = u(1,t) = 0, t \in (0,1], \end{cases} \tag{43}$$

where $0 < \alpha < 1$ and $\frac{\partial^{2\beta}}{\partial|x|^{2\beta}} u(x,t) (1/2 < \beta < 1)$ is the Riesz fractional derivative defined by

$$\frac{\partial^\gamma}{\partial|x|^\gamma} f(x) = -c_\gamma ({}_{-1}^{RL}D_x^\gamma + {}_x^{RL}D_1^\gamma) f(x), \text{ and } c_\gamma = \frac{1}{2\cos\frac{\pi\gamma}{2}}.$$

Similar to the above strategy, let $\tilde{t} = 2t - 1$, and (43) is converted into

$$(1/2)^{-\alpha}\, {}_{-1}^C D_{\tilde{t}}^\alpha \hat{u}(x,\tilde{t}) = -c_\gamma ({}_{-1}^{RL}D_x^\gamma + {}_x^{RL}D_1^\gamma) \hat{u}(x,\tilde{t}) + \hat{f}(x,\tilde{t}), \tag{44}$$

where $\hat{u}(x,\tilde{t}) = u(x, \frac{1}{2} + \frac{1}{2}\tilde{t})$, $\hat{f}(x,\tilde{t}) = f(x, \frac{1}{2} + \frac{1}{2}\tilde{t})$.

For the Riesz fractional diffusion equation (43), we consider the exact solution $u(x,t) = t^{3+\alpha}(x+1)^2(1-x)^2$. The temporal and spatial accuracies are shown in Figure 8 for $t = 1$, where the left column corresponds to $\beta = 0.55$, and the right column to $\beta = 0.95$. The top row shows the temporal accuracies versus M, and the bottom row shows the spatial accuracies versus N.

5.4. Nonlinear fractional differential equations. Now, we consider a nonlinear fractional differential equation below by using our method

$$\begin{aligned} {}_0^C D_t^\alpha y(t) = {} & \frac{40320}{\Gamma(9-\alpha)} t^{8-\alpha} - 3\frac{\Gamma(5+\alpha/2)}{\Gamma(5-\alpha/2)} t^{4-\alpha/2} + \frac{9}{4}\Gamma(\alpha+1) \\ & + \left(\frac{3}{2} t^{\alpha/2} - t^4\right)^3 - [y(t)]^{\frac{3}{2}}, \; 0 < t \le 1, \end{aligned} \tag{45}$$

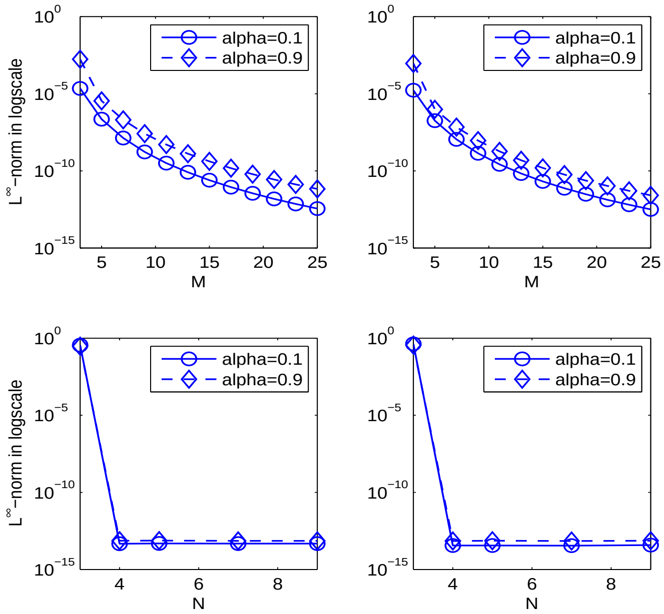

FIGURE 8. The maximum errors of (43) in log-scale. Top row: temporal accuracies; Bottom row: spatial accuracies. Left column: $\beta = 0.55$; Right column: $\beta = 0.95$.

with initial values $y(0) = y'(0) = 0$. Here, the order of fractional derivative $1 < \alpha < 2$. This equation (45) is from [26] and its exact solution is

$$y(t) = t^8 - 3t^{4+\alpha/2} + \frac{9}{4}t^{\alpha}.$$

In order to use our method, the domain $[0, 1]$ is firstly transferred into $[-1, 1]$. Let $\tilde{t} = 2t - 1$. Then, the equation (45) is rewritten into

$$\begin{aligned}(1/2)^{-\alpha}\,{}_{-1}^{\,C}D_{\tilde{t}}^{\alpha}\hat{y}(\tilde{t}) = {} & \frac{40320}{\Gamma(9-\alpha)}\left(\frac{\tilde{t}+1}{2}\right)^{8-\alpha} - 3\frac{\Gamma(5+\alpha/2)}{\Gamma(5-\alpha/2)}\left(\frac{\tilde{t}+1}{2}\right)^{4-\alpha/2} \\ & + \frac{9}{4}\Gamma(\alpha+1) + \left[\frac{3}{2}\left(\frac{\tilde{t}+1}{2}\right)^{\alpha/2} - \left(\frac{\tilde{t}+1}{2}\right)^{4}\right]^{3} - [\hat{y}(\tilde{t})]^{\frac{3}{2}}\end{aligned} \tag{46}$$

in which $\tilde{t} \in (-1, 1)$.

Assume that $\tilde{t}_j (j = 0, 1, \cdots, M)$ are the collocation points on $[-1, 1]$, and that $y_N(\tilde{t})$ is the spectral collocation solution of (46) such that

$$y_N(\tilde{t}) = \sum_{i=0}^{M} y(\tilde{t}_i) l_i(\tilde{t}),$$

where $l_i(\tilde{t})|_{i=0}^{M}$ are the Lagrange interpolation polynomials based on $\tilde{t}_j (j = 0, 1, \cdots, M)$. Let D_{1+r}^{C} be the fractional differentiation matrix with the entries $d_{ij} =$

${}_{-1}^{C}D_{\tilde{t}}^{1+r} l_j(\tilde{t}_i)$ for $r = \alpha - 1$. By the initial conditions,

$$y_N(-1) = \sum_{i=0}^{M} y(\tilde{t}_i) l_i(-1) = 0, \text{ and } y_N'(-1) = \sum_{i=0}^{M} y(\tilde{t}_i) l_i'(-1) = 0,$$

then the other $M-1$ equations are derived from (46) for $y_N(\tilde{t})$ by taking $M-1$ collocation points $\tilde{t}_1, \tilde{t}_2, \cdots, \tilde{t}_{M-1}$. Hence, a closed nonlinear system of equations is obtained which is solved by the Newton iteration method. In addition, noting that

$$l_i'(\tilde{t}) = l_i(\tilde{t}) \sum_{\substack{k=0 \\ k \neq i}}^{M} (\tilde{t} - \tilde{t}_k)^{-1}.$$

The numerical results are shown in Table 1. In order to see the algebraic convergence, we plot the maximum errors in Figure 9 in log-log scale. It shows that the spectral collocation method is algebraically convergent.

TABLE 1. The L^∞−errors for solving the equation (45) by spectral collocation method.

M	$\alpha = 1.1$	$\alpha = 1.9$
8	2.4734e-02	6.2521e-03
16	5.4184e-03	1.5486e-03
32	1.2447e-03	3.8633e-04
64	3.2404e-04	9.6533e-05
128	7.1096e-05	2.3827e-05

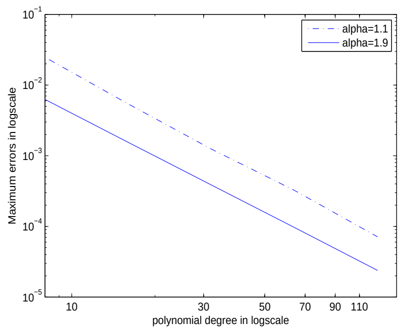

FIGURE 9. The maximum errors of (45) in log-log scale.

5.5. Non-smooth problems. To end this section, we consider a subdiffusion problem with non-smooth data by the spectral collocation method and the corrected backward differentiation formulas (BDFs) proposed in the recent paper [19]. Here, we shall compare the convergence rates and the run-time of these two methods. All the computations are carried out on a personal lapton with 64bit operation system. The problem is expressed by

$$(47) \qquad {}_{0}^{C}D_{t}^{\alpha} u(t,x) - \triangle u(t,x) = f(t,x),\ t > 0,\ 0 < x < 1$$

with the initial conditions $u(0,x) = 0$, and a homogeneous Dirichlet boundary condition, in which $0 < \alpha < 1$, and $\triangle$ designates the Laplacian operator. Here, the source $f(t,x) = 2t^\alpha + \Gamma(1+\alpha)x(1-x)$ is not regular enough in time.

In this example, because the Laplacian is a regular operator and the data in space are all smooth, the approximated solution of the form $\sum_{i=0}^{M}\sum_{j=0}^{N} u_{ij}l_i(t)l_j(x)$ can attain the desired accuracy by the lower number N. Here, we choose $N = 30$ which is enough to obtain higher accuracy in space compared with the time direction. The errors in L^2-norm and CPU time for the cases $\gamma = 0.25, 0.5, 0.75$ are listed in Table 2.

TABLE 2. The L^2-errors and CPU time (sec) for solving the equation (47) versus M with $N = 30$ by spectral collocation method.

M	$\alpha = 0.25$		$\alpha = 0.5$		$\alpha = 0.75$	
	$\|u-u_N\|_{L^2}$	time	$\|u-u_N\|_{L^2}$	time	$\|u-u_N\|_{L^2}$	time
10	5.4532e-05	0.15	2.3786e-05	0.11	5.0307e-06	0.10
20	1.0029e-05	0.12	5.9305-07	0.11	1.2557e-06	0.11
40	1.6007e-06	0.23	5.0310e-07	0.22	3.0839e-07	0.30
80	2.0755e-07	0.64	1.3485e-07	0.64	7.7287e-08	0.64
160	1.6803e-08	3.42	3.3563e-08	3.57	1.9355e-08	3.51

In order to show the efficiency and high convergence rate of the space-time spectral collocation method, we list the errors in L^2-norm and CPU time for the same fractional derivative orders γ in Table 3, by using the corrected BDF2 [19] in temporal discretization and spectral collocation in spatial discretization with the same collocation points as the above space-time spectral collocation method. From Table 2 and Table 3, it can be seen that the space-time spectral collocation method based on the recurrence formulas is still an efficient and highly accurate method even for nonsingular fractional PDEs.

TABLE 3. The L^2-errors and CPU time (sec) for solving the equation (47) versus M with $N = 30$ by spectral collocation method in spatial discretization and corrected BDF2 in temporal discretization with time-step $\tau = 1/M$.

M	$\alpha = 0.25$		$\alpha = 0.5$		$\alpha = 0.75$	
	$\|u-u_N\|_{L^2}$	time	$\|u-u_N\|_{L^2}$	time	$\|u-u_N\|_{L^2}$	time
50	3.5277e-05	0.05	1.3238e-05	0.06	2.7487e-06	0.05
100	1.4844e-05	0.05	4.7061e-06	0.05	8.2912e-07	0.07
200	6.2451e-06	0.08	1.6705e-06	0.07	2.4941e-07	0.09
400	2.6269e-06	0.18	5.9237e-07	0.16	7.4877e-08	0.17
800	1.1048e-06	0.44	2.0989e-07	0.41	2.2443e-08	0.47
1600	4.6460e-07	1.56	7.4322e-08	1.52	6.7180e-09	1.42

6. Conclusion

For fractional differential equations, high-order methods are more complicated than the classical counterparts due to the long-range effect of the fractional derivatives, so that the computational complexity of the fractional derivatives are larger compared with the cases of the integer order. In order to derive a high order scheme, the discretization of the fractional derivative term becomes the largest handicap to be overcome. In this paper, a new algorithm used for computing the fractional derivatives of various types is proposed. The computing schemes for fractional derivatives are derived by recurrence formulas based on the Chebyshev polynomials of the second kind. Base on this algorithm, the spectral collocation method is investigated. Our method is efficient for solving various fractional equations, such as the multi-term fractional equations, the time and/or space fractional diffusion equations, the time-space Riesz fractional diffusion equations, nonlinear fractional differential equations and non-smooth problems. Our method may employ high-degree polynomials to deal with some problems of lower regularity and attain high accuracy. It is worthwhile noting that our method is quite convenient for the analysis of error estimate compared to those using the generalized Jacobi functions.

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Appendix.

Here, we present the proof of Theorem 4.1. This proof follows the line of one of Theorem 3.4 in [36].

Proof of Theorem 4.1. Let $P_j^{a,b}(x)$ be Jacobi polynomials with weighted function $w^{a,b}(x) = (1-x)^a(1+x)^b$. Then, one has (see [27] for details),

$$\int_{-1}^{1} P_m^{a,b}(x)P_n^{a,b}(x)w^{a,b}dx = \delta_{mn}\beta_n^{a,b}, \tag{A.1}$$

where δ_{mn} is the Kronecker delta symbol and

$$\beta_n^{a,b} = \frac{2^{a+b+1}\Gamma(n+a+1)\Gamma(n+b+1)}{(2n+a+b+1)n!\Gamma(n+a+b+1)}.$$

Note that the differential property of the Jacobi polynomials

$$\frac{d^m}{dx^m}P_n^{a,b}(x) = d_{n,m}^{a,b}P_{n-m}^{a+m,b+m}(x),\ d_{n,m}^{a,b} = \frac{\Gamma(n+m+a+b+1)}{2^m\Gamma(n+a+b+1)}, \quad n \geq m. \tag{A.2}$$

Denote by $h_{n,m}^{a,b} = (d_{n,m}^{a,b})^2\beta_{n-m}^{a,b}$.

By (9) and (10), we have

$$\|{}_{-1}^{RL}D_x^\gamma T_n(x)\|^2_{w^{-1/2,2\gamma-1/2}} \leq Cn^{2\gamma}\beta_n^{-1/2,-1/2}, \tag{A.3}$$

$$\|{}_x^{RL}D_1^\gamma T_n(x)\|^2_{w^{2\gamma-1/2,-1/2}} \leq Cn^{2\gamma}\beta_n^{-1/2,-1/2}, \tag{A.4}$$

since $\frac{\Gamma(k+1)}{\Gamma(k-\gamma+1)} = O(k^\gamma)$. Further, it follows that

$$\|{}_{-1}^{RL}D_x^\gamma\phi\|_{w^{a,2\gamma+b}} \leq CN^\gamma\|\phi\|_{w^{a,b}}, \tag{A.5}$$

$$\|{}_x^{RL}D_1^\gamma\phi\|_{w^{2\gamma+a,b}} \leq CN^\gamma\|\phi\|_{w^{a,b}}, \tag{A.6}$$

for any $\phi \in \mathbb{P}_N$.

Let $u \in H^m_{w^{-1/2,-1/2},*}(\Lambda)$, define the orthogonal projection $\Pi_N : L^2 \to \mathbb{P}_N$ such that

$$(\Pi_N u - u, w) = 0, \quad \forall w \in \mathbb{P}_N.$$

Then, $\Pi_N u = \sum_{k=0}^N \hat{u}_n T_n(x)$, where $\hat{u}_n = \frac{1}{\beta_n^{-1/2,-1/2}}(u, T_n)_{w^{-1/2,-1/2}}$. By combining (A.3) with (A.1) and (A.2), we have

$$\begin{aligned}\|{}_{-1}^{RL}D_x^\gamma(\Pi_N u - u)\|^2_{w^{-1/2,2\gamma-1/2}} &\leq C\sum_{n=N+1}^{\infty} n^{2\gamma}|\hat{u}_n|^2\beta_n^{-1/2,-1/2} \\ &= C\sum_{n=N+1}^{\infty}|\hat{u}_n|^2 h_{n,m}^{-\frac12,-\frac12}n^{2\gamma}\frac{\beta_n^{-1/2,-1/2}h_{n,0}^{-\frac12,-\frac12}}{h_{n,m}^{-\frac12,-\frac12}} \\ &\leq CN^{2\gamma-2m}\|\partial_x^m u\|^2_{w^{m-1/2,m-1/2}}, \end{aligned} \tag{A.7}$$

where the fact

$$\frac{h_{n,0}^{-\frac12,-\frac12}}{h_{n,m}^{-\frac12,-\frac12}} = \frac{\Gamma(n)\Gamma(n-m+1)}{\Gamma(n+m)\Gamma(n+1)} = O(n^{-2m})$$

is used. Hence, by (A.5) and (A.7), it yields that

$$\begin{aligned}&\|{}_{-1}^{RL}D_x^\gamma(I_N u - u)\|_{w^{-1/2,2\gamma-1/2}} \\ &\leq \|{}_{-1}^{RL}D_x^\gamma(\Pi_N u - u)\|_{w^{-1/2,2\gamma-1/2}} + \|{}_{-1}^{RL}D_x^\gamma I_N(u - \Pi_N u)\|_{w^{-1/2,2\gamma-1/2}} \\ &\leq CN^{r-m}\|\partial_x^m u\|_{w^{m-1/2,m-1/2}} + CN^\gamma\|I_N(u-\Pi_N u)\|_{w^{-1/2,-1/2}}.\end{aligned} \tag{A.8}$$

Note that

$$\begin{aligned}\|I_N(u-\Pi_N u)\|_{w^{-1/2,-1/2}} &\leq \|\Pi_N u - u\|_{w^{-1/2,-1/2}} + \|I_N u - u\|_{w^{-1/2,-1/2}} \\ &\leq CN^{-m}\|\partial_x^m u\|_{w^{m-1/2,m-1/2}},\end{aligned}$$

this gives the estimation of $\|{}_{-1}^{RL}D_x^{\gamma}(I_N u - u)\|_{w^{-1/2,2\gamma-1/2}}$.

Similarly, the estimation of $\|{}_{x}^{RL}D_1^{\gamma}(I_N u - u)\|_{w^{-1/2,2\gamma-1/2}}$ can be derived. The proof is completed. □

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