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GENERALIZED JACOBI FUNCTIONS AND THEIR APPLICATIONS TO FRACTIONAL DIFFERENTIAL EQUATIONS

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Abstract. In this paper, we consider spectral approximation of fractional differential equations (FDEs). A main ingredient of our approach is to define a new class of generalized Jacobi functions (GJFs), which is intrinsically related to fractional calculus and can serve as natural basis functions for properly designed spectral methods for FDEs. We establish spectral approximation results for these GJFs in weighted Sobolev spaces involving fractional derivatives. We construct efficient GJF-Petrov-Galerkin methods for a class of prototypical fractional initial value problems (FIVPs) and fractional boundary value problems (FBVPs) of general order, and we show that with an appropriate choice of the parameters in GJFs, the resulting linear systems are sparse and well-conditioned. Moreover, we derive error estimates with convergence rates only depending on the smoothness of data, so true spectral accuracy can be attained if the data are smooth enough. The ideas and results presented in this paper will be useful in dealing with more general FDEs involving Riemann-Liouville or Caputo fractional derivatives.

1. Introduction

Fractional differential equations appear in the investigation of transport dynamics in complex systems which are governed by anomalous diffusion and non-exponential relaxation patterns. Related equations of importance are the space/time fractional diffusion equations, the fractional advection-diffusion equations for anomalous diffusion with sources and sinks, the fractional Fokker-Planck equations for anomalous diffusion in an external field, and others. Progress in the last two decades has demonstrated that many phenomena in various fields of science, mathematics, engineering, bioengineering, and economics are more accurately described by involving fractional derivatives. Nowadays, FDEs are emerging as a new powerful tool for modeling many different types of complex systems, i.e.,

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systems with overlapping microscopic and macroscopic scales or systems with long-range time memory and long-range spatial interactions (see, e.g., [7, 8, 15, 25, 26] and the references therein).

There has been a growing interest in the last decades in developing numerical methods for solving FDEs, and a large volume of literature is available on this subject. Generally speaking, the two main difficulties for dealing with FDEs are

(i) fractional derivatives are non-local operators;
(ii) fractional derivatives involve singular kernel/weight functions, and the solutions of FDEs are usually singular near the boundaries.

Most of the existing numerical methods for FDEs are based on finite-difference and finite-element methods (cf. [9, 11, 14, 22–24, 28, 30] and the references therein) which lack the capability to effectively deal with the aforementioned difficulties, as they are based on "local" operations and are not well suited for problems with singular kernels/weights. In particular, due to the non-local nature of the fractional derivatives, they all lead to full and dense matrices which are expensive to calculate and invert. Recently, some interesting ideas have been proposed for overcoming these difficulties. For instance, Wang and Basu [31] proposed a fast finite-difference method by carefully analyzing the structure of the coefficient matrices of the resulting linear systems, and delicately decomposing them into a combination of sparse and structured dense matrices.

Also limited but very promising efforts have been devoted to developing spectral methods for solving FDEs (see, e.g., [19–21, 32]). This appears to be a natural approach, since the spectral method is global, which should be better suited for non-local problems. Most notably, Zayernouri and Karniadakis [32] proposed to use poly-fractonomials, which are eigenfunctions of a fractional Sturm-Liouville operator, as basis functions, leading to sparse matrices for some simple model equations. Preliminary results in [32] showed that this new approach could lead to several orders of magnitude savings in CPU and memory for some model FDEs. However, there is no error analysis available for the approximation properties of poly-fractonomials, and the algorithms therein do not necessarily lead to spectral convergence for problems with smooth data, but non-smooth solution which is typical for FDEs.

The second difficulty is largely ignored in the literature. Typically, the solution and data of an FDE are not in the same type of Sobolev spaces, which is in distinct contrast with usual differential equations. Consequently, they should be approximated by different tools, and the error estimates should be measured in norms of different types of spaces. Indeed, given smooth data, the solution only has limited regularity in the usual Sobolev spaces. However, existing error estimates for FDEs, either finite differences, finite elements, or spectral methods, are mostly based on the usual approach, namely, the errors are estimated in the framework of usual Sobolev spaces. Hence, it is not surprising to see that most existing methods and the related error estimates only lead to poor convergence rates for typical FDEs, unless for manufactured smooth exact solutions.

The purpose of this paper is to develop and analyze efficient spectral methods which can effectively address the above two issues for a class of prototypical FDEs. The main strategies and contributions are highlighted as follows.

- We introduce a new class of GJFs with two parameters, which can be tuned to match singularity of the underlying solution, and simultaneously produce

sparse linear systems. More importantly, such GJFs enjoy attractive fractional calculus properties and remarkable approximability to functions with singular behaviors at boundaries.

- We derive optimal approximation results for these GJFs in properly weighted spaces involving fractional derivatives and obtain error estimates for the proposed GJF-Petrov-Galerkin approaches with convergence rates only depending on smoothness of the data (characterized by usual Sobolev norms). Thus, truly spectral accuracy can be achieved for some model FDEs with sufficiently smooth data.
- We point out that the GJFs, including generalized Jacobi polynomials (GJPs) as special cases, were first introduced in [12, 13] for solutions of usual boundary value problems. Here, we modify the original definition, which opens up new applications in solving FDEs. We also remark that GJFs with parameters in $(0, 1)$ have direct bearing on the Jacobi polyfractonomials in [32]. The major difference lies in that the new GJFs are built upon Jacobi polynomials *with real parameters.*

While we shall only consider some prototypical FIVPs and FBVPs of general order, we position this work as the first but important step towards developing efficient spectral methods for more complicated FDEs involving Riemann-Liouville or Caputo fractional derivatives.

The paper is organized as follows. In the next section, we make necessary preparations by recalling basic properties of Jacobi polynomials with real parameters and introduce the important Bateman fractional integral formula. In Section 3, we define the GJFs and derive their essential properties, particularly, including fractional calculus properties. In Section 4, we establish the approximation results for these GJFs. In Section 5, we construct efficient GJF-Petrov-Galerkin methods for a class of prototypical FDEs, conduct error analysis, and present ample supporting numerical results. In the final section, we extend some important results for the Riemann-Liouville fractional derivative to the Caputo fractional derivative, and we conclude the paper with a few remarks.

2. Preliminaries

In this section, we review basics of fractional integrals and derivatives, and recall relevant properties of the Jacobi polynomials with real parameters. In particular, we introduce the Bateman fractional integral formula, which plays a very important role in the forthcoming algorithm development and analysis.

2.1. **Fractional integrals and derivatives.**

Let $\mathbb{N}$ and $\mathbb{R}$ be the set of positive integers and real numbers, respectively. Denote

$$\mathbb{N}_0 := \{0\} \cup \mathbb{N}, \quad \mathbb{R}^+ := \{a \in \mathbb{R} : a > 0\}, \quad \mathbb{R}_0^+ := \{0\} \cup \mathbb{R}^+. \tag{2.1}$$

We first recall the definitions of fractional integrals and fractional derivatives in the sense of Riemann-Liouville and Caputo (see, e.g., [7, 26]). To fix the idea, we restrict our attention to the interval $\Lambda := (-1, 1)$. It is clear that all formulas and properties can be formulated on a general interval (a, b).

Definition 2.1 (Fractional integrals and derivatives)**.** For $\rho \in \mathbb{R}^+$, the left and right fractional integrals are defined respectively as

$$\begin{aligned} {}_{-1}I_x^\rho v(x) &= \frac{1}{\Gamma(\rho)} \int_{-1}^{x} \frac{v(y)}{(x-y)^{1-\rho}} dy, \quad x \in \Lambda, \\ {}_{x}I_1^\rho v(x) &= \frac{1}{\Gamma(\rho)} \int_{x}^{1} \frac{v(y)}{(y-x)^{1-\rho}} dy, \qquad x \in \Lambda, \end{aligned} \tag{2.2}$$

where $\Gamma(\cdot)$ is the usual Gamma function.

For $s \in [k-1, k)$ with $k \in \mathbb{N}$, the left-hand side Riemann-Liouville fractional derivative of order s is defined by

$${}_{-1}D_x^s v(x) = \frac{1}{\Gamma(k-s)} \frac{d^k}{dx^k} \int_{-1}^{x} \frac{v(y)}{(x-y)^{s-k+1}} dy, \quad x \in \Lambda, \tag{2.3}$$

and the right-hand side Riemann-Liouville fractional derivative of order s is defined by

$${}_{x}D_1^s v(x) = \frac{(-1)^k}{\Gamma(k-s)} \frac{d^k}{dx^k} \int_{x}^{1} \frac{v(y)}{(y-x)^{s-k+1}} dy, \quad x \in \Lambda. \tag{2.4}$$

For $s \in [k-1, k)$ with $k \in \mathbb{N}$, the left-hand side Caputo fractional derivatives of order s is defined by

$${}^{C}_{-1}D_x^s v(x) := \frac{1}{\Gamma(k-s)} \int_{-1}^{x} \frac{v^{(k)}(y)}{(x-y)^{s-k+1}} dy, \quad x \in \Lambda, \tag{2.5}$$

and the right-hand side Caputo fractional derivatives of order s is defined by

$${}^{C}_{x}D_1^s v(x) := \frac{(-1)^k}{\Gamma(k-s)} \int_{x}^{1} \frac{v^{(k)}(y)}{(y-x)^{s-k+1}} dy, \quad x \in \Lambda. \tag{2.6}$$

It is clear that for any $k \in \mathbb{N}_0$,

$${}_{-1}D_x^k = D^k, \quad {}_{x}D_1^k = (-1)^k D^k, \quad \text{where} \quad D^k := d^k/dx^k. \tag{2.7}$$

Thus, we can define the fractional derivatives as

$$\begin{aligned} {}_{-1}D_x^k v(x) &= D^k {}_{-1}I_x^{k-s} v(x), \quad {}_{x}D_1^k v(x) = (-1)^k D^k {}_{x}I_1^{k-s} v(x), \\ {}^{C}_{-1}D_x^k v(x) &= {}_{-1}I_x^{k-s} D^k v(x), \quad {}^{C}_{x}D_1^k v(x) = (-1)^k {}_{x}I_1^{k-s} D^k v(x). \end{aligned} \tag{2.8}$$

According to [7, Thm. 2.14], we have that for any absolutely integrable function v and real $s \geq 0$,

$${}_{-1}D_x^s \, {}_{-1}I_x^s v(x) = v(x), \quad {}_{x}D_1^s \, {}_{x}I_1^s v(x) = v(x) \quad \text{a.e. in } \Lambda. \tag{2.9}$$

The following lemma shows the relationship between the Riemann-Liouville and Caputo fractional derivatives (see, e.g., [26, Ch. 2]).

Lemma 2.1. *For $s \in [k-1, k)$ with $k \in \mathbb{N}$, we have*

$${}_{-1}D_x^s v(x) = {}^{C}_{-1}D_x^s v(x) + \sum_{j=0}^{k-1} \frac{v^{(j)}(-1)}{\Gamma(1+j-s)} (1+x)^{j-s}, \tag{2.10a}$$

$${}_{x}D_1^s v(x) = {}^{C}_{x}D_1^s v(x) + \sum_{j=0}^{k-1} \frac{(-1)^j v^{(j)}(1)}{\Gamma(1+j-s)} (1-x)^{j-s}. \tag{2.10b}$$

Remark 2.1. In the above, the Gamma function with negative, non-integer argument should be understood by the Euler reflection formula (cf. [1]):

$$\Gamma(1+j-s)=\frac{\pi}{\sin(\pi(1+j-s))}\frac{1}{\Gamma(s-j)},\quad s\in(k-1,k),\ \ 1\le j\le k-2.$$

Note that if $s=k-1$, then $\Gamma(1+j-s)=\infty$ for all $0\le j\le k-2$, so the summations in the above reduce to $(\pm1)^{k-1}v^{(k-1)}(\mp1)$, respectively. □

Remark 2.2. Observe immediately from (2.10) that for $s\in[k-1,k)$ with $k\in\mathbb{N}$,

$$\begin{aligned}&{}_{-1}D_x^s v(x)={}_{-1}^{C}D_x^s v(x),\quad \text{if } v^{(j)}(-1)=0,\ \ j=0,\dots,k-1;\\ &{}_{x}D_1^s v(x)={}_{x}^{C}D_1^s v(x),\qquad \text{if } v^{(j)}(1)=0,\ \ j=0,\dots,k-1.\end{aligned}\tag{2.11}$$

□

The rule of fractional integration by parts (see, e.g., [16]) will also be used subsequently.

Lemma 2.2. *For $s\in[k-1,k)$ with $k\in\mathbb{N}$, we have*

$$\big({}_{-1}D_x^s u,v\big)=\big(u,{}_{x}^{C}D_1^s v\big)+\sum_{j=0}^{k-1}(-1)^j v^{(j)}(x)D^{k-j-1}\,{}_{-1}I_x^{k-s}u(x)\Big|_{x=-1}^{x=1},\tag{2.12a}$$

$$\big({}_{x}D_1^s u,v\big)=\big(u,{}_{-1}^{C}D_x^s v\big)+\sum_{j=0}^{k-1}(-1)^{k-j} v^{(j)}(x)D^{k-j-1}\,{}_{x}I_1^{k-s}u(x)\Big|_{x=-1}^{x=1},\tag{2.12b}$$

where $(\cdot,\cdot)$ is the L^2-inner product.

2.2. **Jacobi polynomials with real parameters.** Much of our discussion later will make use of Jacobi polynomials with real parameters. Here, the notation and normalization are in accordance with Szegö [29].

Recall the hypergeometric function (cf. [1])

$${}_2F_1(a,b;c;x)=\sum_{j=0}^{\infty}\frac{(a)_j(b)_j}{(c)_j}\frac{x^j}{j!},\quad |x|<1,\quad a,b,c\in\mathbb{R},\ -c\notin\mathbb{N}_0,\tag{2.13}$$

where the rising factorial in the Pochhammer symbol, for $a\in\mathbb{R}$ and $j\in\mathbb{N}_0$, is defined by

$$(a)_0=1;\quad (a)_j:=a(a+1)\cdots(a+j-1)=\frac{\Gamma(a+j)}{\Gamma(a)},\ \ \text{for } j\ge1.\tag{2.14}$$

If a or b is a negative integer, then the hypergeometric function in (2.13) reduces to a polynomial.

According to [29, (4.21.2)], the Jacobi polynomials with parameters $\alpha,\beta\in\mathbb{R}$ are defined by

(2.15)

$$\begin{aligned}P_n^{(\alpha,\beta)}(x)&=\frac{(\alpha+1)_n}{n!}{}_2F_1\Big(-n,n+\alpha+\beta+1;\alpha+1;\frac{1-x}{2}\Big)\\&=\frac{(\alpha+1)_n}{n!}+\sum_{j=1}^{n-1}\frac{(n+\alpha+\beta+1)_j(\alpha+j+1)\cdots(\alpha+n)}{j!(n-j)!}\Big(\frac{x-1}{2}\Big)^j\\&\quad+\frac{(n+\alpha+\beta+1)_n}{n!}\Big(\frac{x-1}{2}\Big)^n,\quad n\ge1,\end{aligned}$$

and $P_0^{(\alpha,\beta)}(x) \equiv 1$. Note that $P_n^{(\alpha,\beta)}(x)$ *is always a polynomial in* x *for all* $\alpha, \beta \in \mathbb{R}$.

Many properties of the classical Jacobi polynomial (with $\alpha, \beta > -1$) can be extended to the general case (see [29, pp. 62-67]). In particular, there hold

$$P_n^{(\alpha,\beta)}(x) = (-1)^n P_n^{(\beta,\alpha)}(-x); \quad P_n^{(\alpha,\beta)}(1) = \frac{(\alpha+1)_n}{n!}. \tag{2.16}$$

Thus, we have the alternative representation:

$$P_n^{(\alpha,\beta)}(x) = (-1)^n \frac{(\beta+1)_n}{n!} {}_2F_1\Big(-n, n+\alpha+\beta+1; \beta+1; \frac{1+x}{2}\Big), \ \ n \geq 1. \tag{2.17}$$

Observe from (2.15) that the coefficient of x^n is

$$l_n^{(\alpha,\beta)} := \frac{(n+\alpha+\beta+1)_n}{2^n n!}, \tag{2.18}$$

so $\deg(P_n^{(\alpha,\beta)}) < n$, if $(n+\alpha+\beta+1)_n = 0$ for given α, β, that is,

$$m := -(n+\alpha+\beta) \in \mathbb{N} \ \text{ and } \ 1 \leq m \leq n. \tag{2.19}$$

A reduction of the degree of $P_n^{(\alpha,\beta)}(x)$ occurs *if and only if* (2.19) *holds* (cf. [29, p. 64]). Indeed, by [29, (4.22.3)], we have that under (2.19),

$$P_n^{(\alpha,\beta)}(x) = \frac{(\alpha+m)\cdots(\alpha+n)}{m(m+1)\cdots n} P_{m-1}^{(\alpha,\beta)}(x) = \frac{(\alpha+m)_{n-m+1}}{m(m+1)\cdots n} P_{m-1}^{(\alpha,\beta)}(x). \tag{2.20}$$

Therefore, there are two degenerate cases:

$$\deg(P_n^{(\alpha,\beta)}) = m-1, \ \text{if } (\alpha+m)_{n-m+1} \neq 0, \tag{2.21}$$

and

$$P_n^{(\alpha,\beta)}(x) \equiv 0, \ \text{if } m = -(n+\alpha+\beta) \in \mathbb{N}, \ -\alpha \in \mathbb{N} \ \text{ and } \ 1 \leq m \leq -\alpha \leq n. \tag{2.22}$$

Interested readers may refer to [6] for a summary of the degenerate cases of Jacobi polynomials. We particularly look at the Jacobi polynomials with one or both parameters being negative integers, which are associated with the transformation formulas.

- Suppose that $P_n^{(\alpha,\beta)}(x)$ does not vanish identically as in (2.22). $P_n^{(\alpha,\beta)}(1) = 0$ if and only if $-\alpha = l \in \mathbb{N}$ and $1 \leq l \leq n$. Moreover, the zero $x = 1$ has a multiplicity l, and there holds the transformation formula (cf. [29, (4.22.2)]):

$$P_n^{(-l,\beta)}(x) = d_n^{l,\beta} \Big(\frac{x-1}{2}\Big)^l P_{n-l}^{(l,\beta)}(x), \quad n \geq l \geq 1, \quad \beta \in \mathbb{R}, \tag{2.23}$$

  where

$$d_n^{l,\beta} = \frac{(n-l)!(\beta+n-l+1)_l}{n!}. \tag{2.24}$$

- Similarly, for $\beta = -m$, we find from (2.16) and (2.23) that

$$P_n^{(\alpha,-m)}(x) = d_n^{m,\alpha} \Big(\frac{x+1}{2}\Big)^m P_{n-m}^{(\alpha,m)}(x), \quad n \geq m \geq 1, \quad \alpha \in \mathbb{R}. \tag{2.25}$$

- If $\alpha = -l$ and $\beta = -m$ with $l, m \in \mathbb{N}$, we deduce from (2.23)-(2.25) that

$$P_n^{(-l,-m)}(x) = \Big(\frac{x-1}{2}\Big)^l \Big(\frac{x+1}{2}\Big)^m P_{n-l-m}^{(l,m)}(x), \quad n \geq l+m. \tag{2.26}$$

Using the contiguous relation [3, (2.5.15)] and the definition (2.15), one can derive the following recurrence relation: for $\alpha, \beta \in \mathbb{R}$,

$$a_n^{\alpha,\beta} P_{n+1}^{(\alpha,\beta)}(x) = (b_n^{\alpha,\beta} x - c_n^{\alpha,\beta}) P_n^{(\alpha,\beta)}(x) - e_n^{\alpha,\beta} P_{n-1}^{(\alpha,\beta)}(x), \quad n \geq 1, \tag{2.27}$$

where

$$\begin{aligned} a_n^{\alpha,\beta} &= 2(n+1)(n+\alpha+\beta+1)(2n+\alpha+\beta), \\ b_n^{\alpha,\beta} &= (2n+\alpha+\beta)(2n+\alpha+\beta+1)(2n+\alpha+\beta+2), \\ c_n^{\alpha,\beta} &= (\beta^2-\alpha^2)(2n+\alpha+\beta+1), \\ e_n^{\alpha,\beta} &= 2(n+\alpha)(n+\beta)(2n+\alpha+\beta+2). \end{aligned} \tag{2.28}$$

Note that by definition,

$$P_0^{(\alpha,\beta)}(x) = 1, \quad P_1^{(\alpha,\beta)}(x) = \frac{1}{2}(\alpha+\beta+2)x + \frac{1}{2}(\alpha-\beta), \quad \alpha, \beta \in \mathbb{R}.$$

For $\alpha, \beta > -1$, the classical Jacobi polynomials are orthogonal with respect to the Jacobi weight function: $\omega^{(\alpha,\beta)}(x) = (1-x)^\alpha (1+x)^\beta$, namely,

$$\int_{-1}^{1} P_n^{(\alpha,\beta)}(x) P_{n'}^{(\alpha,\beta)}(x) \omega^{(\alpha,\beta)}(x)\, dx = \gamma_n^{(\alpha,\beta)} \delta_{nn'}, \tag{2.29}$$

where $\delta_{nn'}$ is the Dirac Delta symbol, and the normalization constant is given by

$$\gamma_n^{(\alpha,\beta)} = \frac{2^{\alpha+\beta+1}\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}{(2n+\alpha+\beta+1)n!\,\Gamma(n+\alpha+\beta+1)}. \tag{2.30}$$

However, the orthogonality does not carry over to the general case. We refer to [18] and [17, Ch. 3] for details.

2.3. **Bateman fractional integral formula.** We recall the fractional integral formula of hypergeometric functions due to Bateman [5] (also see [3, p. 313]): for real $c, \rho \geq 0$,

$${}_2F_1(a,b;c+\rho;x) = \frac{\Gamma(c+\rho)}{\Gamma(c)\Gamma(\rho)} x^{1-(c+\rho)} \int_0^x t^{c-1}(x-t)^{\rho-1} {}_2F_1(a,b;c;t)\, dt, \quad |x| < 1, \tag{2.31}$$

where the hypergeometric function ${}_2F_1$ is defined in (2.13). Observe from (2.2) that one can use the left-hand side of the fractional integral operator (but the left endpoint 0) to express (2.31).

The following formulas, derived from (2.15) and (2.31) (cf. [29, p. 96]), are indispensable for the subsequent discussion.

Lemma 2.3. *Let $\rho \in \mathbb{R}^+$, $n \in \mathbb{N}_0$, and $x \in \Lambda$.*

(i) *For $\alpha > -1$ and $\beta \in \mathbb{R}$,*

$$(1-x)^{\alpha+\rho} \frac{P_n^{(\alpha+\rho,\beta-\rho)}(x)}{P_n^{(\alpha+\rho,\beta-\rho)}(1)} = \frac{\Gamma(\alpha+\rho+1)}{\Gamma(\alpha+1)\Gamma(\rho)} \int_x^1 \frac{(1-y)^\alpha}{(y-x)^{1-\rho}} \frac{P_n^{(\alpha,\beta)}(y)}{P_n^{(\alpha,\beta)}(1)}\, dy. \tag{2.32}$$

(ii) *For $\alpha \in \mathbb{R}$ and $\beta > -1$,*

$$(1+x)^{\beta+\rho} \frac{P_n^{(\alpha-\rho,\beta+\rho)}(x)}{P_n^{(\beta+\rho,\alpha-\rho)}(1)} = \frac{\Gamma(\beta+\rho+1)}{\Gamma(\beta+1)\Gamma(\rho)} \int_{-1}^x \frac{(1+y)^\beta}{(x-y)^{1-\rho}} \frac{P_n^{(\alpha,\beta)}(y)}{P_n^{(\beta,\alpha)}(1)}\, dy. \tag{2.33}$$

Remark 2.3. The formulas (2.32)-(2.33) can be found in several classical books on orthogonal polynomials, but it appears that their derivation is not well described. In fact, taking $a = -n, b = n + \alpha + \beta + 1, c = \alpha + 1$ and $t = (1 - y)/2$ in (2.31), we obtain the formula (2.32) from (2.15). Similarly, (2.33) follows from (2.16) and (2.32). □

Using the notation in Definition 2.1 and working out the constants by (2.16), we can rewrite the formulas in Lemma 2.3 as follows.

Lemma 2.4. *Let* $\rho \in \mathbb{R}^+$, $n \in \mathbb{N}_0$, *and* $x \in \Lambda$.

- *For* $\alpha > -1$ *and* $\beta \in \mathbb{R}$,

$$ {}_xI_1^\rho\big\{(1-x)^\alpha P_n^{(\alpha,\beta)}(x)\big\} = \frac{\Gamma(n+\alpha+1)}{\Gamma(n+\alpha+\rho+1)}(1-x)^{\alpha+\rho}P_n^{(\alpha+\rho,\beta-\rho)}(x). \tag{2.34}$$

- *For* $\alpha \in \mathbb{R}$ *and* $\beta > -1$,

$$ {}_{-1}I_x^\rho\big\{(1+x)^\beta P_n^{(\alpha,\beta)}(x)\big\} = \frac{\Gamma(n+\beta+1)}{\Gamma(n+\beta+\rho+1)}(1+x)^{\beta+\rho}P_n^{(\alpha-\rho,\beta+\rho)}(x). \tag{2.35}$$

Thanks to (2.9), we obtain from Lemma 2.4 the following useful "inverse" rules.

Lemma 2.5. *Let* $s \in \mathbb{R}^+$, $n \in \mathbb{N}_0$, *and* $x \in \Lambda$.

- *For* $\alpha > -1$ *and* $\beta \in \mathbb{R}$,

$$ {}_xD_1^s\big\{(1-x)^{\alpha+s}P_n^{(\alpha+s,\beta-s)}(x)\big\} = \frac{\Gamma(n+\alpha+s+1)}{\Gamma(n+\alpha+1)}(1-x)^\alpha P_n^{(\alpha,\beta)}(x). \tag{2.36}$$

- *For* $\alpha \in \mathbb{R}$ *and* $\beta > -1$,

$$ {}_{-1}D_x^s\big\{(1+x)^{\beta+s}P_n^{(\alpha-s,\beta+s)}(x)\big\} = \frac{\Gamma(n+\beta+s+1)}{\Gamma(n+\beta+1)}(1+x)^\beta P_n^{(\alpha,\beta)}(x). \tag{2.37}$$

Observe that if $\alpha = 0$ in (2.36), the fractional derivative operator ${}_xD_1^s$ takes $(1-x)^s P_n^{(s,\beta-s)}(x)$ to the polynomial $P_n^{(0,\beta)}(x)$. Conversely, if $\alpha + s = k \in \mathbb{N}_0$, ${}_xD_1^s$ takes the polynomial $(1-x)^k P_n^{(k,\beta-s)}(x)$ to $(1-x)^{k-s}P_n^{(k-s,\beta)}(x)$. Such remarkable properties are essential for efficient spectral algorithms to be developed later.

In the forthcoming section, we show that these non-polynomial functions are intimately related to the generalized Jacobi functions introduced in [13]. Moreover, the Jacobi poly-fractonomials first introduced in [32] also have direct bearing on these basis functions when $s \in (0, 1)$.

3. Generalized Jacobi functions

In this section, we modify two subclasses of GJFs defined in [13], leading to the new basis functions, which are still referred to as GJFs. We demonstrate in Section 5 that spectral algorithms using GJFs as basis functions produce spectrally accurate solutions for a class of prototypical fractional differential equations.

3.1. Definition of GJFs.

Definition 3.1 (Generalized Jacobi functions)**.** Define

$$ {}^+J_n^{(-\alpha,\beta)}(x) := (1-x)^\alpha P_n^{(\alpha,\beta)}(x), \quad \text{for } \alpha > -1, \ \beta \in \mathbb{R}, \tag{3.1}$$

and

$$ {}^-J_n^{(\alpha,-\beta)}(x) := (1+x)^\beta P_n^{(\alpha,\beta)}(x), \quad \text{for } \alpha \in \mathbb{R}, \ \beta > -1, \tag{3.2}$$

for all $x \in \Lambda$ and $n \in \mathbb{N}_0$.

Remark 3.1. Note that the so-defined GJFs modified the classical Jacobi polynomials in the range of $-1 < \alpha, \beta < 1$. □

Recall the GJFs introduced in [13, (2.7)]:

(3.3)
$$j_n^{(\alpha,\beta)}(x) = \begin{cases} (1-x)^{-\alpha}(1+x)^{-\beta} P_{\hat{n}}^{(-\alpha,-\beta)}(x), & (\alpha,\beta) \in \aleph_1, \ \ \hat{n} = n - [-\alpha] - [-\beta], \\ (1-x)^{-\alpha} P_{\hat{n}}^{(-\alpha,\beta)}(x), & (\alpha,\beta) \in \aleph_2, \ \ \hat{n} = n - [-\alpha], \\ (1+x)^{-\beta} P_{\hat{n}}^{(\alpha,-\beta)}(x), & (\alpha,\beta) \in \aleph_3, \ \ \hat{n} = n - [-\beta], \\ P_n^{(\alpha,\beta)}(x), & (\alpha,\beta) \in \aleph_4, \end{cases}$$

where $[a]$ denotes the maximum integer $\le a$, and

$$\aleph_1 = \{(\alpha,\beta) : \alpha, \beta \le -1\}, \quad \aleph_2 = \{(\alpha,\beta) : \alpha \le -1, \ \beta > -1\},$$
$$\aleph_3 = \{(\alpha,\beta) : \alpha > -1, \ \beta \le -1\}, \quad \aleph_4 = \{(\alpha,\beta) : \alpha, \beta > -1\}.$$

We elaborate below on the connection and difference between the new GJFs and the GJFs defined in (3.3).

- Comparing (3.1)-(3.2) with (3.3), we find

(3.4)
$$\begin{aligned} {}^{+}J_n^{(-\alpha,\beta)}(x) &= j_{n+[\alpha]}^{(-\alpha,\beta)}(x), \quad \text{if } \ \alpha \ge 1, \ \ \beta > -1, \\ {}^{-}J_n^{(\alpha,-\beta)}(x) &= j_{n+[\beta]}^{(\alpha,-\beta)}(x), \quad \text{if } \ \alpha > -1, \ \ \beta \ge 1. \end{aligned}$$

- By (2.23)-(2.25), we find from (3.1)-(3.2) that for any $\alpha > -1, k \in \mathbb{N}_0$ and $n \ge k$,

(3.5)
$$\begin{aligned} {}^{+}J_n^{(-\alpha,-k)}(x) &= 2^{-k} d_n^{k,\alpha} (1-x)^{\alpha} (1+x)^k P_{n-k}^{(\alpha,k)}(x), \\ {}^{-}J_n^{(-k,-\alpha)}(x) &= (-1)^k 2^{-k} d_n^{k,\alpha} (1-x)^k (1+x)^{\alpha} P_{n-k}^{(k,\alpha)}(x), \end{aligned}$$

which, compared with (3.3), implies that for $\alpha \ge 1$ and $n \ge k \ge 1$,

(3.6)
$${}^{+}J_n^{(-\alpha,-k)}(x) = 2^{-k} d_n^{k,\alpha} j_{n+[\alpha]}^{(-\alpha,-k)}(x), \quad {}^{-}J_n^{(-k,-\alpha)}(x) = (-1)^k 2^{-k} d_n^{k,\alpha} j_{n+[\alpha]}^{(-k,-\alpha)}(x).$$

Here, the constant $d_n^{k,\alpha}$ is defined in (2.24).

We see that we modified the definition of GJFs in [13] for the parameters in the ranges other than those specified in (3.4) and (3.6). Indeed, this opens up new applicability of the GJFs in solving fractional differential equations (see Section 5).

3.2. **Properties of GJFs.** One verifies readily from (2.16) and Definition 3.1 that

$$ {}^{+}J_n^{(-\alpha,\beta)}(-x) = (-1)^n \, {}^{-}J_n^{(\beta,-\alpha)}(x), \quad \alpha > -1, \ \ \beta \in \mathbb{R}, \tag{3.7}$$

and there holds the reflection property

$$ {}^{+}J_n^{(-\alpha,-\alpha)}(x) = (1-x^2)^{\alpha} \, {}^{-}J_n^{(\alpha,\alpha)}(x), \quad -1 < \alpha < 1. \tag{3.8}$$

We derive from (2.27) and (3.1) directly that for $\alpha, \beta \in \mathbb{R}$,

(3.9)
$$\begin{aligned} &a_n^{\alpha,\beta} \, {}^{+}J_{n+1}^{(-\alpha,\beta)}(x) = \big(b_n^{\alpha,\beta} x - c_n^{\alpha,\beta}\big) \, {}^{+}J_n^{(-\alpha,\beta)}(x) - e_n^{\alpha,\beta} \, {}^{+}J_{n-1}^{(-\alpha,\beta)}(x), \ \ n \ge 1, \\ &{}^{+}J_0^{(-\alpha,\beta)}(x) = (1-x)^{\alpha}, \quad {}^{+}J_1^{(-\alpha,\beta)}(x) = \big((\alpha+\beta+2)x + \alpha - \beta\big)(1-x)^{\alpha}/2, \end{aligned}$$

where $a_n^{\alpha,\beta}, b_n^{\alpha,\beta}, c_n^{\alpha,\beta}$, and $e_n^{\alpha,\beta}$ are defined in (2.28). A similar property holds for ${}^{-}J_n^{(\alpha,-\beta)}(x)$.

We now study the orthogonality of GJFs. It follows straightforwardly from (2.29) and Definition 3.1 that for $\alpha, \beta > -1$,

$$\begin{aligned}\int_{-1}^{1} {}^{+}J_n^{(-\alpha,\beta)}(x)\,{}^{+}J_{n'}^{(-\alpha,\beta)}(x)\,\omega^{(-\alpha,\beta)}(x)\,dx \\ = \int_{-1}^{1} {}^{-}J_n^{(\alpha,-\beta)}(x)\,{}^{-}J_{n'}^{(\alpha,-\beta)}(x)\,\omega^{(\alpha,-\beta)}(x)\,dx = \gamma_n^{(\alpha,\beta)}\delta_{nn'},\end{aligned} \tag{3.10}$$

where $\gamma_n^{(\alpha,\beta)}$ is defined in (2.30). Similarly, by (2.29) and (3.5), we have that for $\alpha > -1$ and $k \in \mathbb{N}$,

$$\begin{aligned}&\int_{-1}^{1} {}^{+}J_n^{(-\alpha,-k)}(x)\,{}^{+}J_{n'}^{(-\alpha,-k)}(x)\,\omega^{(-\alpha,-k)}(x)\,dx \\ &\quad = \int_{-1}^{1} {}^{-}J_n^{(-k,-\alpha)}(x)\,{}^{-}J_{n'}^{(-k,-\alpha)}(x)\,\omega^{(-k,-\alpha)}(x)\,dx = \gamma_n^{(\alpha,-k)}\delta_{nn'}, \quad n, n' \ge k,\end{aligned} \tag{3.11}$$

where we used the fact

$$\gamma_n^{(\alpha,-k)} = 2^{-2k}(d_n^{k,\alpha})^2\gamma_{n-k}^{(\alpha,k)}.$$

Next, we discuss the fractional calculus properties of GJFs. The following fractional derivative formulas can be derived straightforwardly from Lemma 2.5 and Definition 3.1.

Theorem 3.1. *Let $s \in \mathbb{R}^+$, $n \in \mathbb{N}_0$, and $x \in \Lambda$.*

- *For $\alpha > s - 1$ and $\beta \in \mathbb{R}$,*

$${}_xD_1^s\big\{{}^{+}J_n^{(-\alpha,\beta)}(x)\big\} = \frac{\Gamma(n+\alpha+1)}{\Gamma(n+\alpha-s+1)}\,{}^{+}J_n^{(-\alpha+s,\beta+s)}(x). \tag{3.12}$$

- *For $\alpha \in \mathbb{R}$ and $\beta > s - 1$,*

$${}_{-1}D_x^s\big\{{}^{-}J_n^{(\alpha,-\beta)}(x)\big\} = \frac{\Gamma(n+\beta+1)}{\Gamma(n+\beta-s+1)}\,{}^{-}J_n^{(\alpha+s,-\beta+s)}(x). \tag{3.13}$$

Some remarks on Theorem 3.1 are in order.

- If $\alpha - s > -1$ and $\beta + s > -1$ with $s \in \mathbb{R}^+$, then by (3.10) and (3.12) $\big\{{}_xD_1^s\,{}^{+}J_n^{(-\alpha,\beta)}\big\}$ are mutually orthogonal with respect to the weight function $\omega^{(-\alpha+s,\beta+s)}(x)$. Similarly, $\big\{{}_{-1}D_x^s\,{}^{-}J_n^{(\alpha,-\beta)}\big\}$ are mutually orthogonal with respect to $\omega^{(\alpha+s,-\beta+s)}(x)$, when $\alpha + s > -1$ and $\beta - s > -1$.
- A very important special case of (3.12) is that for $\alpha > 0$ and $\beta \in \mathbb{R}$,

$${}_xD_1^\alpha\big\{{}^{+}J_n^{(-\alpha,\beta)}(x)\big\} = \frac{\Gamma(n+\alpha+1)}{n!}\,{}^{+}J_n^{(0,\alpha+\beta)}(x) = \frac{\Gamma(n+\alpha+1)}{n!}P_n^{(0,\alpha+\beta)}(x). \tag{3.14}$$

Similarly, by (3.13), we have that for $\alpha \in \mathbb{R}$ and real $\beta > 0$,

$${}_{-1}D_x^\beta\big\{{}^{-}J_n^{(\alpha,-\beta)}(x)\big\} = \frac{\Gamma(n+\beta+1)}{n!}P_n^{(\alpha+\beta,0)}(x). \tag{3.15}$$

These two formulas imply that performing a suitable order of fractional derivatives on GJFs leads to polynomials.

The analysis of the approximability of GJFs essentially relies on the orthogonality of fractional derivatives of GJFs. Recall the derivative formula of the classical Jacobi polynomials (see, e.g., [27, p. 72]): for $\alpha, \beta > -1$ and $n \geq l$,

(3.16)
$$D^l P_n^{(\alpha,\beta)}(x) = \kappa_{n,l}^{(\alpha,\beta)} P_{n-l}^{(\alpha+l,\beta+l)}(x), \quad \text{where } \kappa_{n,l}^{(\alpha,\beta)} := \frac{\Gamma(n+\alpha+\beta+l+1)}{2^l \Gamma(n+\alpha+\beta+1)}.$$

Noting that ${}_xD_1^{s+l} = (-1)^l D^l {}_xD_1^s$ and ${}_{-1}D_x^{s+l} = D^l {}_{-1}D_x^s$ for $s \in \mathbb{R}^+$ and $l \in \mathbb{N}$, we derive from (2.29) and (3.14)-(3.16) the following orthogonality.

- For $\alpha > 0$ and $\alpha + \beta > -1$,

$$\int_{-1}^{1} {}_xD_1^{\alpha+l} {}^{+}J_n^{(-\alpha,\beta)}(x)\ {}_xD_1^{\alpha+l} {}^{+}J_{n'}^{(-\alpha,\beta)}(x)\, \omega^{(l,\alpha+\beta+l)}(x)\, dx = h_{n,l}^{(\alpha,\beta)} \delta_{nn'}, \quad n, n' \geq l \geq 0, \tag{3.17}$$

where

$$\begin{aligned} h_{n,l}^{(\alpha,\beta)} &:= \frac{\Gamma^2(n+\alpha+1)}{(n!)^2} \big(\kappa_{n,l}^{(0,\alpha+\beta)}\big)^2 \gamma_{n-l}^{(l,\alpha+\beta+l)} \\ &= \frac{2^{\alpha+\beta+1}\Gamma^2(n+\alpha+1)\,\Gamma(n+\alpha+\beta+l+1)}{(2n+\alpha+\beta+1)\,n!\,(n-l)!\,\Gamma(n+\alpha+\beta+1)}. \end{aligned} \tag{3.18}$$

- For $\alpha + \beta > -1$ and $\beta > 0$,

$$\int_{-1}^{1} {}_{-1}D_x^{\beta+l} {}^{-}J_n^{(\alpha,-\beta)}(x)\ {}_{-1}D_x^{\beta+l} {}^{-}J_{n'}^{(\alpha,-\beta)}(x)\, \omega^{(\alpha+\beta+l,l)}(x)\, dx = h_{n,l}^{(\beta,\alpha)} \delta_{nn'}, \quad n, n' \geq l \geq 0. \tag{3.19}$$

Another attractive property of GJFs is that they are eigenfunctions of fractional Sturm-Liouville-type equations. To show this, we define the fractional Sturm-Liouville-type operators:

$$\begin{aligned} {}^{+}\mathcal{L}_{\alpha,\beta}^{2s} u &:= \omega^{(\alpha,-\beta)}\, {}_{-1}D_x^s \big\{\omega^{(-\alpha+s,\beta+s)}\, {}_xD_1^s\, u\big\}; \\ {}^{-}\mathcal{L}_{\alpha,\beta}^{2s} u &:= \omega^{(-\alpha,\beta)}\, {}_xD_1^s \big\{\omega^{(\alpha+s,-\beta+s)}\, {}_{-1}D_x^s\, u\big\}. \end{aligned} \tag{3.20}$$

Theorem 3.2. *Let $s \in \mathbb{R}^+$, $n \in \mathbb{N}_0$, and $x \in \Lambda$.*

- *For $\alpha > s - 1$ and $\beta > -1$,*

$${}^{+}\mathcal{L}_{\alpha,\beta}^{2s} {}^{+}J_n^{(-\alpha,\beta)}(x) = \lambda_{n,s}^{(\alpha,\beta)} {}^{+}J_n^{(-\alpha,\beta)}(x), \tag{3.21}$$

where

$$\lambda_{n,s}^{(\alpha,\beta)} := \frac{\Gamma(n+\alpha+1)}{\Gamma(n+\alpha-s+1)} \frac{\Gamma(n+\beta+s+1)}{\Gamma(n+\beta+1)}. \tag{3.22}$$

- *For $\alpha > -1$ and $\beta > s - 1$,*

$${}^{-}\mathcal{L}_{\alpha,\beta}^{2s} {}^{-}J_n^{(\alpha,-\beta)}(x) = \lambda_{n,s}^{(\beta,\alpha)} {}^{-}J_n^{(\alpha,-\beta)}(x). \tag{3.23}$$

Proof. By Definition 3.1 and (3.12), we have that for $\alpha > s - 1$,

$$\begin{aligned} &(1-x)^{-\alpha+s}(1+x)^{\beta+s}\, {}_xD_1^s \big\{{}^{+}J_n^{(-\alpha,\beta)}(x)\big\} \\ &\quad = \frac{\Gamma(n+\alpha+1)}{\Gamma(n+\alpha-s+1)} (1+x)^{\beta+s} P_n^{(\alpha-s,\beta+s)}(x). \end{aligned} \tag{3.24}$$

Applying ${}_{-1}D_x^s$ on both sides of the above identity and tracking the constants, we derive from (2.37) that for $\beta > -1$,

$$\begin{aligned}{}_{-1}D_x^s\big\{\omega^{(-\alpha+s,\beta+s)}(x)\,{}_xD_1^s\big\{{}^{+}J_n^{(-\alpha,\beta)}(x)\big\}\big\} &= \lambda_{n,s}^{(\alpha,\beta)}\,(1+x)^{\beta}P_n^{(\alpha,\beta)}(x)\\ &= \lambda_{n,s}^{(\alpha,\beta)}\,\omega^{(-\alpha,\beta)}(x)\,{}^{+}J_n^{(-\alpha,\beta)}(x).\end{aligned}$$

This yields (3.21).

Property (3.23) can be proved in a very similar fashion. □

Remark 3.2. The above results can be viewed as an extension of the standard Sturm-Liouville problems of GJFs to the fractional derivative case. In [13], we showed that GJFs defined therein are the eigenfunctions of the standard Sturm-Liouville problems. □

Remark 3.3. We derive immediately from (3.22) and Stirling's formula (see (4.26) below) that for fixed s, α, β,

$$\lambda_{n,s}^{(\alpha,\beta)} = O(n^{2s}), \quad \text{for } n \gg 1.$$

When $s \to 1$, this recovers the $O(n^2)$ growth of eigenvalues of the standard Sturm-Liouville problem. □

Note that the fractional Sturm-Liouville operators defined in (3.20) are not self-adjoint in general. However, when $s \in (0,1)$, the singular fractional Sturm-Liouville problems are self-adjoint.

Corollary 3.1. *Let $s \in (0,1)$, $n \in \mathbb{N}_0$, and $x \in \Lambda$.*

- *For $0 < \alpha < s$ and $\beta > -s$, we have that in* (3.21),

$$^{+}\mathcal{L}_{\alpha,\beta}^{2s}\,{}^{+}J_n^{(-\alpha,\beta)} = \omega^{(\alpha,-\beta)}\,{}_{-1}D_x^s\big\{\omega^{(-\alpha+s,\beta+s)}\,{}_x^CD_1^s\,{}^{+}J_n^{(-\alpha,\beta)}\big\}, \tag{3.25}$$

and

$$\begin{aligned}&\big({}^{+}\mathcal{L}_{\alpha,\beta}^{2s}\,{}^{+}J_n^{(-\alpha,\beta)},\,{}^{+}J_m^{(-\alpha,\beta)}\big)_{\omega^{(-\alpha,\beta)}} = \big({}_x^CD_1^s\,{}^{+}J_n^{(-\alpha,\beta)},\,{}_x^CD_1^s\,{}^{+}J_m^{(-\alpha,\beta)}\big)_{\omega^{(-\alpha-s,\beta+s)}}\\ &= \big({}^{+}J_n^{(-\alpha,\beta)},\,{}^{+}\mathcal{L}_{\alpha,\beta}^{2s}\,{}^{+}J_m^{(-\alpha,\beta)}\big)_{\omega^{(-\alpha,\beta)}} = \lambda_{n,s}^{(\alpha,\beta)}\gamma_n^{(-\alpha,\beta)}\delta_{nm}.\end{aligned} \tag{3.26}$$

- *Similarly, for $\alpha > -s$ and $0 < \beta < s$, we have that in* (3.23),

$$^{-}\mathcal{L}_{\alpha,\beta}^{2s}\,{}^{-}J_n^{(\alpha,-\beta)} = \omega^{(-\alpha,\beta)}\,{}_xD_1^s\big\{\omega^{(\alpha+s,-\beta+s)}\,{}_{-1}^CD_x^s\,{}^{-}J_n^{(\alpha,-\beta)}\big\}, \tag{3.27}$$

and

$$\begin{aligned}&\big({}^{-}\mathcal{L}_{\alpha,\beta}^{2s}\,{}^{-}J_n^{(\alpha,-\beta)},\,{}^{-}J_m^{(\alpha,-\beta)}\big)_{\omega^{(\alpha,-\beta)}} = \big({}_{-1}^CD_x^s\,{}^{-}J_n^{(\alpha,-\beta)},\,{}_{-1}^CD_x^s\,{}^{-}J_m^{(\alpha,-\beta)}\big)_{\omega^{(\alpha+s,-\beta-s)}}\\ &= \big({}^{-}J_n^{(\alpha,-\beta)},\,{}^{-}\mathcal{L}_{\alpha,\beta}^{2s}\,{}^{-}J_m^{(\alpha,-\beta)}\big)_{\omega^{(\alpha,-\beta)}} = \lambda_{n,s}^{(\beta,\alpha)}\gamma_n^{(\alpha,-\beta)}\delta_{nm}.\end{aligned} \tag{3.28}$$

Proof. We just prove the results for ${}^{+}J_n^{(-\alpha,\beta)}(x)$. For $\alpha > 0$ and $s \in (0,1)$, since ${}^{+}J_n^{(-\alpha,\beta)}(1) = 0$, we find from (2.11) that ${}_xD_1^s$ can be replaced by ${}_x^CD_1^s$. Accordingly, (3.25) follows from (3.21) immediately.

We now show the fractional integration by parts can get through. By (2.35) and (3.24),

$${}_{-1}I_x^{1-s}\big\{\omega^{(-\alpha+s,\beta+s)}\,{}_x^CD_1^s\,{}^{+}J_n^{(-\alpha,\beta)}\big\} = \tilde{d}_{n,s}^{\alpha,\beta}\,(1+x)^{\beta+1}P_n^{(\alpha-1,\beta+1)}(x), \tag{3.29}$$

where the constant $\tilde{d}_{n,s}^{\alpha,\beta}$ can be worked out. Clearly, it vanishes at $x=-1$. On the other hand, ${}^{+}J_m^{(-\alpha,\beta)}(1)=0$. Therefore, we can perform the rule (2.12a) to obtain the second identity in (3.26). The orthogonality follows from (3.10) and (3.25).

The results for ${}^{-}J_n^{(\alpha,-\beta)}(x)$ can be derived similarly. □

3.3. **Relation with Jacobi poly-fractonomials.** In a very recent paper, Zayernouri and Karniadakis [32] introduced a family of Jacobi poly-fractonomials (JPFs), which were defined as the eigenfunctions of a singular factional Sturm-Liouville problem.

Definition 3.2 (Jacobi poly-fractonomials [32])**.** For $\mu\in(0,1)$, the Jacobi poly-fractonomials of order μ are defined as follows.

- For $-1<\alpha<2-\mu$ and $-1<\beta<\mu-1$,

$$ {}^{(1)}\mathcal{P}_n^{(\alpha,\beta,\mu)}(x)=(1+x)^{\mu-(\beta+1)}P_{n-1}^{(\alpha+1-\mu,\mu-(\beta+1))}(x),\quad n\in\mathbb{N}. \tag{3.30}$$

- For $-1<\alpha<\mu-1$ and $-1<\beta<2-\mu$,

$$ {}^{(2)}\mathcal{P}_n^{(\alpha,\beta,\mu)}(x)=(1-x)^{\mu-(\alpha+1)}P_{n-1}^{(\mu-(\alpha+1),\beta+1-\mu)}(x),\quad n\in\mathbb{N}. \tag{3.31}$$

As shown in [32, Thm. 4.2], the left JPFs are eigenfunctions of the singular fractional Sturm-Liouville equation:

$$\begin{aligned} &{}_xD_1^{\mu}\big\{\omega^{(\alpha+1,\beta+1)}(x)\ {}_{-1}^{C}D_x^{\mu}\{{}^{(1)}\mathcal{P}_n^{(\alpha,\beta,\mu)}(x)\}\big\}\\ &\qquad={}^{(1)}\lambda_n^{(\alpha,\beta,\mu)}\,\omega^{(\alpha+1-\mu,\beta+1-\mu)}(x)\,{}^{(1)}\mathcal{P}_n^{(\alpha,\beta,\mu)}(x), \end{aligned} \tag{3.32}$$

where

$${}^{(1)}\lambda_n^{(\alpha,\beta,\mu)}=\frac{\Gamma(n+\alpha+1)\Gamma(n+\mu-\beta-1)}{\Gamma(n-\beta-1)\Gamma(n-\mu+\alpha+1)},\quad n\geq 1.$$

The right JPFs satisfy a similar equation.

The relation below follows from (3.1)-(3.2) and (3.30)-(3.31):

$$ {}^{(1)}\mathcal{P}_n^{(\alpha,\beta,\mu)}(x)={}^{-}J_{n-1}^{(\alpha+1-\mu,\beta+1-\mu)}(x),\quad {}^{(2)}\mathcal{P}_n^{(\alpha,\beta,\mu)}(x)={}^{+}J_{n-1}^{(\alpha+1-\mu,\beta+1-\mu)}(x). \tag{3.33}$$

Observe that with the parameters $\{\mu,\alpha+1-\mu,\mu-(\beta+1)\}$ in place of $\{s,\alpha,\beta\}$ in (3.27), we obtain (3.32) exactly. However, the range of the parameters is $\alpha>-1$ and $-1<\beta<1-\mu$, so the condition on α is relaxed as opposite to that for (3.30). Indeed, the difference between the range of α is not surprising, as the GJFs here and JPFs in [32] are defined by different means.

4. Approximation by generalized Jacobi functions

The main concern of this section is to show that approximation by GJFs leads to truly spectral convergence for functions in properly weighted Sobolev spaces involving fractional derivatives. Such approximation results play a crucial role in the analysis of spectral methods for fractional differential equations (see Section 5).

For simplicity of presentation, we only provide the detailed analysis for $\{{}^{+}J_n^{(-\alpha,\beta)}\}$ as the results can be extended to $\{{}^{-}J_n^{(\alpha,-\beta)}\}$ straightforwardly, thanks to (3.7). In the first place, we highlight some special GJFs of particular interest.

- In view of the fractional factor $(1-x)^{\alpha}$, we have that for $\alpha>0$ and $\beta\in\mathbb{R}$,

$$ D^l\,{}^{+}J_n^{(-\alpha,\beta)}(1)=0,\quad \text{for } l=0,1,\ldots,[\alpha]-1. \tag{4.1}$$

Suppose that $P_n^{(\alpha,\beta)}(x)$ does not degenerate for all $n \geq 0$ (cf. (2.19)-(2.22)). Then we can naturally impose the one-sided boundary conditions: $u^{(l)}(1) = 0$ for $l = 0, 1, \ldots, [\alpha]-1$. More importantly, the basis matches the singularity of the solution for prototypical FIVPs, thanks to the fractional factor $(1-x)^\alpha$. Moreover, we can choose the parameter β (e.g., $\beta = -\alpha$) so that under the GJF basis, the resulting linear system can be sparse and well conditioned (see Section 5). However, it is noteworthy that the choice of β does not affect the approximability of the basis.

- For $\alpha > 0$, $\beta = -[\alpha]$ and $n \geq [\alpha]$, we find from (3.5) that

$$D^l\, {}^{+}J_n^{(-\alpha,-[\alpha])}(\pm 1) = 0, \quad \text{for} \quad l = 0, 1, \ldots, [\alpha] - 1, \tag{4.2}$$

which allows us to deal with the two-sided boundary condition $u^{(l)}(\pm 1) = 0$, and to match the singularity of the underlying solution (see Section 5).

We introduce some notation to be used later. Let $\mathcal{P}_N$ be the set of all algebraic (real-valued) polynomials of degree at most N. Let $\varpi(x) > 0$, $x \in \Lambda$, be a generic weight function. The weighted space $L^2_\varpi(\Lambda)$ is defined as in Adams [2] with inner product and norm

$$(u, v)_\varpi = \int_\Lambda u(x)v(x)\varpi(x)dx, \quad \|u\|_\varpi = (u, u)_\varpi^{1/2}.$$

If $\varpi \equiv 1$, we omit the weight function in the notation. In what follows, the Sobolev space $H^1(\Lambda)$ is also defined as usual.

4.1. **Approximation results for GJFs $\{{}^{+}J_n^{(-\alpha,\beta)}\}$.** In view of the applications, we restrict the parameters to the set

$${}^{+}\Upsilon^{\alpha,\beta} := \big\{(\alpha, \beta) \,:\, \alpha > 0, \;\; \alpha + \beta > -1\big\}, \tag{4.3}$$

which we further split into three disjoint subsets:

$$\begin{aligned}
{}^{+}\Upsilon_1^{\alpha,\beta} &:= \big\{(\alpha, \beta) \,:\, \alpha > 0, \; \beta > -1\big\};\\
{}^{+}\Upsilon_2^{\alpha,\beta} &:= \big\{(\alpha, \beta) \,:\, \alpha > 0, \; -\alpha - 1 < \beta = -k \leq -1, \; k \in \mathbb{N}\big\};\\
{}^{+}\Upsilon_3^{\alpha,\beta} &:= \big\{(\alpha, \beta) \,:\, \alpha > 0, \; -\alpha - 1 < \beta < -1, \; -\beta \notin \mathbb{N}\big\}.
\end{aligned} \tag{4.4}$$

4.1.1. *Case I:* $(\alpha, \beta) \in {}^{+}\Upsilon_1^{\alpha,\beta} \cup {}^{+}\Upsilon_2^{\alpha,\beta}$. Let us first consider $(\alpha, \beta) \in {}^{+}\Upsilon_1^{\alpha,\beta}$. In this case, we define the finite-dimensional fractional-polynomial space:

$${}^{+}\mathcal{F}_N^{(-\alpha,\beta)}(\Lambda) = \big\{\phi = (1-x)^\alpha \psi \,:\, \psi \in \mathcal{P}_N\big\} = \mathrm{span}\big\{{}^{+}J_n^{(-\alpha,\beta)} \,:\, 0 \leq n \leq N\big\}. \tag{4.5}$$

By the orthogonality (3.10), we can expand any $u \in L^2_{\omega^{(-\alpha,\beta)}}(\Lambda)$ as

$$u(x) = \sum_{n=0}^{\infty} \hat{u}_n^{(-\alpha,\beta)}\, {}^{+}J_n^{(-\alpha,\beta)}(x), \;\; \text{where} \;\; \hat{u}_n^{(-\alpha,\beta)} = \frac{1}{\gamma_n^{(\alpha,\beta)}} \int_{-1}^{1} u\, {}^{+}J_n^{(-\alpha,\beta)} \omega^{(-\alpha,\beta)}\, dx, \tag{4.6}$$

and there holds the Parseval identity

$$\|u\|^2_{\omega^{(-\alpha,\beta)}} = \sum_{n=0}^{\infty} \gamma_n^{(\alpha,\beta)} \big|\hat{u}_n^{(-\alpha,\beta)}\big|^2. \tag{4.7}$$

Consider the $L^2_{\omega^{(-\alpha,\beta)}}$-orthogonal projection upon ${}^{+}\mathcal{F}_N^{(-\alpha,\beta)}(\Lambda)$, defined by

$$\big({}^{+}\pi_N^{(-\alpha,\beta)} u - u, v_N\big)_{\omega^{(-\alpha,\beta)}} = 0, \quad \forall\, v_N \in {}^{+}\mathcal{F}_N^{(-\alpha,\beta)}(\Lambda). \tag{4.8}$$

By definition, we have

$$({}^{+}\pi_N^{(-\alpha,\beta)}u)(x) = \sum_{n=0}^{N} \hat{u}_n^{(-\alpha,\beta)}\, {}^{+}J_n^{(-\alpha,\beta)}(x). \tag{4.9}$$

Remark 4.1. In the above, we have used the completeness of $\{{}^{+}J_n^{(-\alpha,\beta)}\}$ in $L^2_{\omega^{(-\alpha,\beta)}}(\Lambda)$. Here, we provide a justification for this. Note that for any $u \in L^2_{\omega^{(-\alpha,\beta)}}(\Lambda)$, we have $(1-x)^{-\alpha}u \in L^2_{\omega^{(\alpha,\beta)}}(\Lambda)$. For $(\alpha,\beta) \in {}^{+}\Upsilon_1^{\alpha,\beta}$, i.e., $\alpha > 0, \beta > -1$, $\{P_n^{(\alpha,\beta)}\}_{n\geq 0}$ are mutually orthogonal and complete in $L^2_{\omega^{(\alpha,\beta)}}(\Lambda)$, so we can uniquely expand

$$(1-x)^{-\alpha}u(x) = \sum_{n=0}^{\infty} \tilde{v}_n^{(\alpha,\beta)} P_n^{(\alpha,\beta)}(x), \tag{4.10}$$

where by (2.29), (3.1), and (4.6),

$$\begin{aligned}\tilde{v}_n^{(\alpha,\beta)} &= \frac{1}{\gamma_n^{(\alpha,\beta)}} \int_{-1}^{1} (1-x)^{-\alpha} u(x) P_n^{(\alpha,\beta)}(x) \omega^{(\alpha,\beta)}(x) dx \\ &= \frac{1}{\gamma_n^{(\alpha,\beta)}} \int_{-1}^{1} u(x) {}^{+}J_n^{(-\alpha,\beta)}(x) \omega^{(-\alpha,\beta)}(x) dx = \hat{u}_n^{(-\alpha,\beta)}.\end{aligned}$$

Multiplying both sides of (4.10) by $(1-x)^{\alpha}$, we obtain the unique representation (4.6). Hence, we can claim the completeness of $\{{}^{+}J_n^{(-\alpha,\beta)}\}$ in $L^2_{\omega^{(-\alpha,\beta)}}(\Lambda)$. □

We now consider $(\alpha,\beta) \in {}^{+}\Upsilon_2^{\alpha,\beta}$. In this case, we modify (4.5) as

$${}^{+}\mathcal{F}_N^{(-\alpha,-k)}(\Lambda) = \big\{\phi = (1-x)^{\alpha}\psi \,:\, \psi \in \mathcal{P}_N \text{ such that } \psi^{(l)}(-1) = 0,\ 0 \leq l \leq k-1\big\}, \tag{4.11}$$

which incorporates the homogeneous boundary conditions at $x = -1$. Thanks to (3.5), we have

$${}^{+}\mathcal{F}_N^{(-\alpha,-k)}(\Lambda) = \operatorname{span}\big\{{}^{+}J_n^{(-\alpha,-k)}(x) \,:\, k \leq n \leq N\big\}. \tag{4.12}$$

In view of the orthogonality (3.11), we have an expansion like (4.6), that is, for any $u \in L^2_{\omega^{(-\alpha,-k)}}(\Lambda)$,

$$u(x) = \sum_{n=k}^{\infty} \hat{u}_n^{(-\alpha,-k)}\, {}^{+}J_n^{(-\alpha,-k)}(x), \tag{4.13}$$

where

$$\hat{u}_n^{(-\alpha,-k)} = \frac{1}{\gamma_n^{(\alpha,-k)}} \int_{-1}^{1} u(x)\, {}^{+}J_n^{(-\alpha,-k)}(x)\, \omega^{(-\alpha,-k)}(x)\, dx. \tag{4.14}$$

Note that the identity (4.7) also holds for this expansion. The partial sum

$${}^{+}\pi_N^{(-\alpha,-k)}u(x) = \sum_{n=k}^{N} \hat{u}_n^{(-\alpha,-k)}\, {}^{+}J_n^{(-\alpha,-k)}(x), \tag{4.15}$$

is the $L^2_{\omega^{(-\alpha,-k)}}$-orthogonal projection upon ${}^{+}\mathcal{F}_N^{(-\alpha,-k)}(\Lambda)$, namely,

$$\big({}^{+}\pi_N^{(-\alpha,-k)}u - u, v_N\big)_{\omega^{(-\alpha,-k)}} = 0, \quad \forall\, v_N \in {}^{+}\mathcal{F}_N^{(-\alpha,-k)}(\Lambda). \tag{4.16}$$

Remark 4.2. Like Remark 4.1, we need to justify $\{{}^{+}J_n^{(-\alpha,-k)}\}$ is complete in $L^2_{\omega^{(-\alpha,-k)}}(\Lambda)$. For $(\alpha,\beta)\in {}^{+}\Upsilon_2^{\alpha,\beta}$ (so $\alpha>0$ and $-\beta=k\in\mathbb{N}$), one verifies that for any $u\in L^2_{\omega^{(-\alpha,-k)}}(\Lambda)$, we have $\omega^{(-\alpha,-k)}u\in L^2_{\omega^{(\alpha,k)}}(\Lambda)$, which can be uniquely expressed in series of $\{P_{n-k}^{(\alpha,k)}\}_{n\geq k}$. In view of (3.5), we can show the completeness of $\{{}^{+}J_n^{(-\alpha,-k)}\}$ in $L^2_{\omega^{(-\alpha,-k)}}(\Lambda)$ in the same fashion as in Remark 4.1. □

Remark 4.3. It is worthwhile to point out that for $(\alpha,\beta)\in {}^{+}\Upsilon_1^{\alpha,\beta}\cup {}^{+}\Upsilon_2^{\alpha,\beta}$, we have

$$\big({}_xD_1^{\alpha+l}({}^{+}\pi_N^{(-\alpha,\beta)}u-u),D^l w_N\big)_{\omega^{(l,\alpha+\beta+l)}}=0,\quad \forall\, w_N\in\mathcal{P}_N, \tag{4.17}$$

for all $l\in\mathbb{N}_0$. Notice that

$$({}^{+}\pi_N^{(-\alpha,\beta)}u-u)(x)=\sum_{n=N+1}^{\infty}\hat{u}_n^{(-\alpha,\beta)}\,{}^{+}J_n^{(-\alpha,\beta)}(x),$$

and $\mathcal{P}_N=\operatorname{span}\big\{P_n^{(0,\alpha+\beta)}\,:\,0\leq n\leq N\big\}$. Using the property ${}_xD_1^{\alpha+l}=(-1)^lD^l\,{}_xD_1^{\alpha}$ for $\alpha>0$ and $l\in\mathbb{N}$, we obtain (4.17) from (3.14), (3.16), and the orthogonality of the classical Jacobi polynomials (cf. (2.29)). □

To characterise the regularity of u, we introduce the non-uniformly Jacobi weighted space involving fractional derivatives:

$${}^{+}\mathcal{B}^m_{\alpha,\beta}(\Lambda):=\big\{u\in L^2_{\omega^{(-\alpha,\beta)}}(\Lambda)\,:\,{}_xD_1^{\alpha+l}u\in L^2_{\omega^{(l,\alpha+\beta+l)}}(\Lambda)\quad \text{for } 0\leq l\leq m\big\},\quad m\in\mathbb{N}_0. \tag{4.18}$$

By (3.17) and (4.6) or (4.13), we have that for $(\alpha,\beta)\in {}^{+}\Upsilon_1^{\alpha,\beta}\cup {}^{+}\Upsilon_2^{\alpha,\beta}$ and $l\in\mathbb{N}_0$,

$$\big\|{}_xD_1^{\alpha+l}u\big\|^2_{\omega^{(l,\alpha+\beta+l)}}=\sum_{n=\tilde{l}}^{\infty}h_{n,\tilde{l}}^{(\alpha,\beta)}\big|\hat{u}_n^{(\alpha,\beta)}\big|^2, \tag{4.19}$$

where $\tilde{l}=l$ for $(\alpha,\beta)\in {}^{+}\Upsilon_1^{\alpha,\beta}$; $\tilde{l}=\max\{l,k\}$ for $(\alpha,\beta)\in {}^{+}\Upsilon_2^{\alpha,\beta}$, and $h_{n,\tilde{l}}^{(\alpha,\beta)}$ is defined in (3.18).

The main result on the projection errors for these two cases is stated as follows.

Theorem 4.1. *Let $(\alpha,\beta)\in {}^{+}\Upsilon_1^{\alpha,\beta}\cup {}^{+}\Upsilon_2^{\alpha,\beta}$, and let $u\in {}^{+}\mathcal{B}^m_{\alpha,\beta}(\Lambda)$ with $m\in\mathbb{N}_0$.*

- *For $0\leq l\leq m\leq N$,*

$$\begin{aligned}&\big\|{}_xD_1^{\alpha+l}({}^{+}\pi_N^{(-\alpha,\beta)}u-u)\big\|_{\omega^{(l,\alpha+\beta+l)}}\\&\quad\leq N^{(l-m)/2}\sqrt{\frac{(N-m+1)!}{(N-l+1)!}}\,\big\|{}_xD_1^{\alpha+m}u\big\|_{\omega^{(m,\alpha+\beta+m)}}.\end{aligned} \tag{4.20}$$

  In particular, if m is fixed, then

$$\big\|{}_xD_1^{\alpha+l}({}^{+}\pi_N^{(-\alpha,\beta)}u-u)\big\|_{\omega^{(l,\alpha+\beta+l)}}\leq cN^{l-m}\big\|{}_xD_1^{\alpha+m}u\big\|_{\omega^{(m,\alpha+\beta+m)}}. \tag{4.21}$$

- *For $0\leq m\leq N$, we also have the $L^2_{\omega^{(-\alpha,\beta)}}$-estimates*

$$\big\|{}^{+}\pi_N^{(-\alpha,\beta)}u-u\big\|_{\omega^{(-\alpha,\beta)}}\leq cN^{-\alpha}\sqrt{\frac{(N-m+1)!}{(N+m+1)!}}\,\big\|{}_xD_1^{\alpha+m}u\big\|_{\omega^{(m,\alpha+\beta+m)}}. \tag{4.22}$$

In particular, if m is fixed, then

$$\big\|{}^{+}\pi_N^{(-\alpha,\beta)}u-u\big\|_{\omega^{(-\alpha,\beta)}}\le cN^{-(\alpha+m)}\big\|{}_xD_1^{\alpha+m}u\big\|_{\omega^{(m,\alpha+\beta+m)}}. \tag{4.23}$$

Here, $c\approx 1$ for $N\gg 1$.

Proof. By (4.6) (or (4.13)), (4.8) (or (4.16)) and (4.19),

$$\begin{aligned}&\big\|{}_xD_1^{\alpha+l}({}^{+}\pi_N^{(-\alpha,\beta)}u-u)\big\|^2_{\omega^{(l,\alpha+\beta+l)}}\\ &\quad=\sum_{n=N+1}^{\infty}h_{n,l}^{(\alpha,\beta)}\big|\hat{u}_n^{(\alpha,\beta)}\big|^2=\sum_{n=N+1}^{\infty}\frac{h_{n,l}^{(\alpha,\beta)}}{h_{n,m}^{(\alpha,\beta)}}h_{n,m}^{(\alpha,\beta)}\big|\hat{u}_n^{(\alpha,\beta)}\big|^2\\ &\quad\le\frac{h_{N+1,l}^{(\alpha,\beta)}}{h_{N+1,m}^{(\alpha,\beta)}}\big\|{}_xD_1^{\alpha+m}u\big\|^2_{\omega^{(m,\alpha+\beta+m)}}.\end{aligned} \tag{4.24}$$

We now estimate the constant factor. By (2.14), (3.18) and a direct calculation, we find that for $0\le l\le m\le N$,

$$\begin{aligned}\frac{h_{N+1,l}^{(\alpha,\beta)}}{h_{N+1,m}^{(\alpha,\beta)}}&=\frac{\Gamma(N+\alpha+\beta+l+2)}{\Gamma(N+\alpha+\beta+m+2)}\frac{(N-m+1)!}{(N-l+1)!}\\ &=\frac{1}{(N+\alpha+\beta+2+l)\cdots(N+\alpha+\beta+1+m)}\frac{(N-m+1)!}{(N-l+1)!}\\ &\le N^{l-m}\frac{(N-m+1)!}{(N-l+1)!},\end{aligned} \tag{4.25}$$

where we used the fact that $\alpha+\beta>-1$. Therefore, the estimate (4.20) follows from (4.24)-(4.25) immediately.

We now turn to (4.21). Let us recall the property of the Gamma function (see [1, (6.1.38)]):

$$\Gamma(x+1)=\sqrt{2\pi}x^{x+1/2}\exp\Big(-x+\frac{\theta}{12x}\Big),\quad\forall\,x>0,\ \ 0<\theta<1. \tag{4.26}$$

We can show that for any constant $a,b\in\mathbb{R}$, $n\in\mathbb{N}$, $n+a>1$ and $n+b>1$ (see [33, Lemma 2.1]),

$$\frac{\Gamma(n+a)}{\Gamma(n+b)}\le\nu_n^{a,b}n^{a-b}, \tag{4.27}$$

where

$$\nu_n^{a,b}=\exp\Big(\frac{a-b}{2(n+b-1)}+\frac{1}{12(n+a-1)}+\frac{(a-b)^2}{n}\Big). \tag{4.28}$$

Using the property $\Gamma(n+1)=n!$ and (4.27), we find that for $m\le N$,

$$\frac{(N-m+1)!}{(N-l+1)!}\le\nu_N^{2-m,2-l}N^{l-m}, \tag{4.29}$$

where $\nu_N^{2-m,2-l}\approx 1$ for fixed m and $N\gg 1$. Thus, we obtain (4.21) from (4.20) immediately.

The $L^2_{\omega^{(-\alpha,\beta)}}$-estimates can be obtained by using the same argument. We sketch the derivation below. By (4.7) and (4.19),

(4.30)
$$\begin{aligned}\big\|{}^{+}\pi_N^{(-\alpha,\beta)}u-u\big\|^2_{\omega^{(-\alpha,\beta)}}&=\sum_{n=N+1}^{\infty}\gamma_n^{(\alpha,\beta)}\,\big|\hat{u}_n^{(\alpha,\beta)}\big|^2\\&\le\frac{\gamma_{N+1}^{(\alpha,\beta)}}{h_{N+1,m}^{(\alpha,\beta)}}\sum_{n=N+1}^{\infty}h_{n,m}^{(\alpha,\beta)}\,\big|\hat{u}_n^{(\alpha,\beta)}\big|^2\le\frac{\gamma_{N+1}^{(\alpha,\beta)}}{h_{N+1,m}^{(\alpha,\beta)}}\big\|{}_xD_1^{\alpha+m}u\big\|^2_{\omega^{(m,\alpha+\beta+m)}}.\end{aligned}$$

Working out the constants by (2.30) and (3.18), we use (4.27) again to get that

(4.31)
$$\begin{aligned}\frac{\gamma_{N+1}^{(\alpha,\beta)}}{h_{N+1,m}^{(\alpha,\beta)}}&=\frac{\Gamma(N+\beta+2)}{\Gamma(N+\alpha+2)}\frac{\Gamma(N+m+2)}{\Gamma(N+\alpha+\beta+m+2)}\frac{(N-m+1)!}{(N+m+1)!}\\&\le\nu_N^{\alpha+2,\beta+2}N^{\beta-\alpha}\;\nu_N^{2,\alpha+\beta+2}(N+m)^{-(\alpha+\beta)}\frac{(N-m+1)!}{(N+m+1)!}\\&\le cN^{-2(\alpha+m)}\quad(\text{if } m \text{ is fixed}).\end{aligned}$$

This ends the proof. □

Remark 4.4. We see from the above estimates that an optimal order of convergence can be attained for approximation of u by its orthogonal projection ${}^{+}\pi_N^{(-\alpha,\beta)}u$ in both $L^2_{\omega^{(-\alpha,\beta)}}(\Lambda)$ and ${}^{+}\mathcal{B}^l_{\alpha,\beta}(\Lambda)$, when u belongs to a properly weighted space involving proper orders of fractional derivatives. □

4.1.2. *Case II:* $(\alpha,\beta)\in{}^{+}\Upsilon_3^{\alpha,\beta}$. In this case, the main difficulty resides in that the GJFs $\{{}^{+}J_n^{(-\alpha,\beta)}\}$ are no longer orthogonal. In what follows, we adopt a different route to derive the approximation results. For any u such that ${}_xD_1^{\alpha}u\in L^2_{\omega^{(0,\alpha+\beta)}}(\Lambda)$, it admits the unique Jacobi series expansion

$$ {}_xD_1^{\alpha}u(x)=\sum_{n=0}^{\infty}\hat{v}_n^{(0,\alpha+\beta)}P_n^{(0,\alpha+\beta)}(x), \tag{4.32}$$

where by orthogonality (2.29)

$$ \hat{v}_n^{(0,\alpha+\beta)}=\frac{1}{\gamma_n^{(0,\alpha+\beta)}}\int_{-1}^{1}{}_xD_1^{\alpha}u(x)\;P_n^{(0,\alpha+\beta)}(x)\,(1+x)^{\alpha+\beta}\,dx. \tag{4.33}$$

From the definition of the $L^2_{\omega^{(0,\alpha+\beta)}}$-orthogonal projection: $\Pi_N^{(0,\alpha+\beta)}:L^2_{\omega^{(0,\alpha+\beta)}}(\Lambda)\to\mathcal{P}_N$, we have

$$ \big(\Pi_N^{(0,\alpha+\beta)}({}_xD_1^{\alpha}u)-{}_xD_1^{\alpha}u,v_N\big)_{\omega^{(0,\alpha+\beta)}}=0,\quad\forall\,v_N\in\mathcal{P}_N, \tag{4.34}$$

and

$$ \Pi_N^{(0,\alpha+\beta)}({}_xD_1^{\alpha}u)(x)=\sum_{n=0}^{N}\hat{v}_n^{(0,\alpha+\beta)}P_n^{(0,\alpha+\beta)}(x). \tag{4.35}$$

Let ${}^{+}\mathcal{F}_N^{(-\alpha,\beta)}(\Lambda)$ be the finite-dimensional space as defined in (4.5), but for $(\alpha,\beta)\in\Upsilon_3^{\alpha,\beta}$.

Lemma 4.1. *Let $(\alpha,\beta)\in\Upsilon_3^{\alpha,\beta}$, i.e., $\alpha>0,-\alpha-1<\beta<-1$ and $-\beta\notin\mathbb{N}$. Then for any u such that ${}_xD_1^\alpha u\in L^2_{\omega^{(0,\alpha+\beta)}}(\Lambda)$, there exists a unique $u_N=:{}^+\pi_N^{(-\alpha,\beta)}u\in{}^+\mathcal{F}_N^{(-\alpha,\beta)}(\Lambda)$ such that*

$$\Pi_N^{(0,\alpha+\beta)}({}_xD_1^\alpha u)(x)={}_xD_1^\alpha({}^+\pi_N^{(-\alpha,\beta)}u)(x) \tag{4.36}$$

and

$$\big({}_xD_1^\alpha({}^+\pi_N^{(-\alpha,\beta)}u-u),v_N\big)_{\omega^{(0,\alpha+\beta)}}=0,\quad\forall\, v_N\in\mathcal{P}_N. \tag{4.37}$$

Proof. From the coefficients $\big\{\hat v_n^{(0,\alpha+\beta)}\big\}_{n=0}^N$ in (4.33), we construct

$$u_N(x)=\sum_{n=0}^N\frac{n!\,\hat v_n^{(0,\alpha+\beta)}}{\Gamma(n+\alpha+1)}{}^+J_n^{(-\alpha,\beta)}(x)\in{}^+\mathcal{F}_N^{(-\alpha,\beta)}(\Lambda). \tag{4.38}$$

Acting ${}_xD_1^\alpha$ on both sides, we obtain from (3.14) and (4.35) that

$${}_xD_1^\alpha u_N(x)=\sum_{n=0}^N\hat v_n^{(0,\alpha+\beta)}P_n^{(0,\alpha+\beta)}(x)=\Pi_N^{(0,\alpha+\beta)}({}_xD_1^\alpha u)(x).$$

Note that the expansion in (4.33) is unique, so we specifically denote u_N by ${}^+\pi_N^{(-\alpha,\beta)}u$, and (4.36) is shown.

The property (4.37) is a direct consequence of (4.34) and (4.36). □

With Lemma 4.1 at our disposal, we can obtain the following error estimates.

Theorem 4.2. *Let $(\alpha,\beta)\in\Upsilon_3^{\alpha,\beta}$, i.e., $\alpha>0,-\alpha-1<\beta<-1$ and $-\beta\notin\mathbb{N}$, and let ${}^+\pi_N^{(-\alpha,\beta)}$ be defined in Lemma 4.1. Suppose that ${}_xD_1^{\alpha+l}u\in L^2_{\omega^{(l,\alpha+\beta+l)}}(\Lambda)$ with $0\le l\le m\le N$. Then we have*

$$\big\|{}_xD_1^\alpha({}^+\pi_N^{(-\alpha,\beta)}u-u)\big\|_{\omega^{(0,\alpha+\beta)}}\le N^{-m/2}\sqrt{\frac{(N-m+1)!}{(N+1)!}}\big\|{}_xD_1^{\alpha+m}u\big\|_{\omega^{(m,\alpha+\beta+m)}}. \tag{4.39}$$

In particular, if m is fixed, we have

$$\big\|{}_xD_1^\alpha({}^+\pi_N^{(-\alpha,\beta)}u-u)\big\|_{\omega^{(0,\alpha+\beta)}}\le cN^{-m}\big\|{}_xD_1^{\alpha+m}u\big\|_{\omega^{(m,\alpha+\beta+m)}}, \tag{4.40}$$

where the constant $c\approx1$ for $N\gg1$.

Proof. Using the relation (4.36), we derive from (2.29), (4.32), and (4.35) that

$$\begin{aligned}\big\|{}_xD_1^\alpha({}^+\pi_N^{(-\alpha,\beta)}u-u)\big\|^2_{\omega^{(0,\alpha+\beta)}}&=\big\|\Pi_N^{(0,\alpha+\beta)}({}_xD_1^\alpha u)-{}_xD_1^\alpha u\big\|^2_{\omega^{(0,\alpha+\beta)}}\\&=\sum_{n=N+1}^\infty\gamma_n^{(0,\alpha+\beta)}\big|\hat v_n^{(0,\alpha+\beta)}\big|^2.\end{aligned} \tag{4.41}$$

We find from (2.29), (3.16), and (4.32) that

$$\big\|{}_xD_1^{\alpha+m}u\big\|^2_{\omega^{(m,\alpha+\beta+m)}}=\sum_{n=m}^\infty\mu_{n,m}^{(0,\alpha+\beta)}\big|\hat v_n^{(0,\alpha+\beta)}\big|^2, \tag{4.42}$$

where for $n\ge m$,

$$\mu_{n,m}^{(0,\alpha+\beta)}=\big(\kappa_{n,m}^{(0,\alpha+\beta)}\big)^2\gamma_{n-m}^{(m,\alpha+\beta+m)}=\frac{2^{\alpha+\beta+1}n!\,\Gamma(n+\alpha+\beta+m+1)}{(2n+\alpha+\beta+1)\,(n-m)!\,\Gamma(n+\alpha+\beta+1)}. \tag{4.43}$$

In view of the above facts, we work out the constants by using (2.30) and obtain

$$\begin{aligned}\big\|{}_xD_1^{\alpha}({}^{+}\pi_N^{(-\alpha,\beta)}u-u)\big\|^2_{\omega^{(0,\alpha+\beta)}} &\le \frac{\gamma_{N+1}^{(0,\alpha+\beta)}}{\mu_{N+1,m}^{(0,\alpha+\beta)}}\big\|{}_xD_1^{\alpha+m}u\big\|^2_{\omega^{(m,\alpha+\beta+m)}}\\ &= \frac{1}{(N+\alpha+\beta+2)_m}\frac{(N+1-m)!}{(N+1)!}\big\|{}_xD_1^{\alpha+m}u\big\|^2_{\omega^{(m,\alpha+\beta+m)}}\\ &\le N^{-m}\frac{(N+1-m)!}{(N+1)!}\big\|{}_xD_1^{\alpha+m}u\big\|^2_{\omega^{(m,\alpha+\beta+m)}}.\end{aligned}\tag{4.44}$$

This yields (4.39). For fixed m, we apply (4.27) to deal with the above factorials and derive (4.40) immediately. □

4.2. **Approximation results for GJFs $\{{}^{-}J_n^{(\alpha,-\beta)}\}$.** Thanks to (3.7), the estimates established in the previous subsection can be extended to $\{{}^{-}J_n^{(\alpha,-\beta)}\}$ straightforwardly. To avoid repetition, we sketch the corresponding results.

Like (4.3), we define the parameter set

$${}^{-}\Upsilon^{\alpha,\beta}:=\big\{(\alpha,\beta)\,:\,\beta>0,\ \ \alpha+\beta>-1\big\},\tag{4.45}$$

which we split into three disjoint subsets:

$$\begin{aligned}{}^{-}\Upsilon_1^{\alpha,\beta}&:=\big\{(\alpha,\beta)\,:\,\beta>0,\ \alpha>-1\big\};\\ {}^{-}\Upsilon_2^{\alpha,\beta}&:=\big\{(\alpha,\beta)\,:\,\beta>0,\ -\beta-1<\alpha=-k\le -1,\ k\in\mathbb{N}\big\};\\ {}^{-}\Upsilon_3^{\alpha,\beta}&:=\big\{(\alpha,\beta)\,:\,\beta>0,\ -\beta-1<\alpha<-1,\ -\alpha\notin\mathbb{N}\big\}.\end{aligned}\tag{4.46}$$

Consider the $L^2_{\omega^{(\alpha,-\beta)}}$-orthogonal projection: ${}^{-}\pi_N^{(\alpha,-\beta)}u\in{}^{-}\mathcal{F}_N^{(\alpha,-\beta)}(\Lambda)$ for $(\alpha,\beta)\in{}^{-}\Upsilon_1^{\alpha,\beta}\cup{}^{-}\Upsilon_2^{\alpha,\beta}$, where the notation is defined in a fashion similar to that in the previous subsection. In this context, we define

$$\begin{aligned}{}^{-}\mathcal{B}^m_{\alpha,\beta}(\Lambda):=\big\{u\in L^2_{\omega^{(\alpha,-\beta)}}(\Lambda)\,:\,{}_{-1}D_x^{\beta+l}u\in L^2_{\omega^{(\alpha+\beta+l,l)}}(\Lambda)\\ \text{for }\ 0\le l\le m\big\},\quad m\in\mathbb{N}_0.\end{aligned}\tag{4.47}$$

Following the argument as in the proof of Theorem 4.1, we can derive the following error estimates.

Theorem 4.3. *Let $(\alpha,\beta)\in{}^{-}\Upsilon_1^{\alpha,\beta}\cup{}^{-}\Upsilon_2^{\alpha,\beta}$, and let $u\in{}^{-}\mathcal{B}^m_{\alpha,\beta}(\Lambda)$ with $m\in\mathbb{N}_0$.*

- *For $0\le l\le m\le N$,*

$$\begin{aligned}&\big\|{}_{-1}D_x^{\beta+l}({}^{-}\pi_N^{(\alpha,-\beta)}u-u)\big\|_{\omega^{(\alpha+\beta+l,l)}}\\ &\qquad\le N^{(l-m)/2}\sqrt{\frac{(N-m+1)!}{(N-l+1)!}}\,\big\|{}_{-1}D_x^{\beta+m}u\big\|_{\omega^{(\alpha+\beta+m,m)}}.\end{aligned}\tag{4.48}$$

  In particular, if m is fixed, we have

$$\big\|{}_{-1}D_x^{\beta+l}({}^{-}\pi_N^{(\alpha,-\beta)}u-u)\big\|_{\omega^{(\alpha+\beta+l,l)}}\le cN^{l-m}\,\big\|{}_{-1}D_x^{\beta+m}u\big\|_{\omega^{(\alpha+\beta+m,m)}}.\tag{4.49}$$

- *For $0\le m\le N$, we also have the $L^2_{\omega^{(\alpha,-\beta)}}$-estimates*

$$\big\|{}^{-}\pi_N^{(\alpha,-\beta)}u-u\big\|_{\omega^{(\alpha,-\beta)}}\le cN^{-\beta}\sqrt{\frac{(N-m+1)!}{(N+m+1)!}}\,\big\|{}_{-1}D_x^{\beta+m}u\big\|_{\omega^{(\alpha+\beta+m,m)}}.\tag{4.50}$$

In particular, if m is fixed, then

$$\left\|{}^{-}\pi_N^{(\alpha,-\beta)}u-u\right\|_{\omega^{(\alpha,-\beta)}}\le cN^{-(\beta+m)}\left\|{}_{-1}D_x^{\beta+m}u\right\|_{\omega^{(\alpha+\beta+m,m)}}. \tag{4.51}$$

Here, $c\approx 1$ for $N\gg 1$.

Next, we consider $(\alpha,\beta)\in {}^{-}\Upsilon_3^{\alpha,\beta}$. For ${}_{-1}D_x^{\beta}u\in L^2_{\omega^{(\alpha+\beta,0)}}(\Lambda)$, we define the operator ${}^{-}\Pi_N^{(\alpha,-\beta)}$ similarly as that in Lemma 4.1. Following the lines as in the proof of Theorem 4.2, we can obtain the following estimates.

Theorem 4.4. *Let $(\alpha,\beta)\in {}^{-}\Upsilon_3^{\alpha,\beta}$. Suppose that ${}_{-1}D_x^{\beta+l}u\in L^2_{\omega^{(\alpha+\beta+l,l)}}(\Lambda)$ with $0\le l\le m\le N$. Then we have*

$$\left\|{}_{-1}D_x^{\beta}({}^{-}\pi_N^{(\alpha,-\beta)}u-u)\right\|_{\omega^{(\alpha+\beta,0)}}\le N^{-m/2}\sqrt{\frac{(N-m+1)!}{(N+1)!}}\left\|{}_{-1}D_x^{\beta+m}u\right\|_{\omega^{(\alpha+\beta+m,m)}}. \tag{4.52}$$

In particular, if m is fixed, we have

$$\left\|{}_{-1}D_x^{\beta}({}^{-}\pi_N^{(\alpha,-\beta)}u-u)\right\|_{\omega^{(\alpha+\beta,0)}}\le cN^{-m}\left\|{}_{-1}D_x^{\beta+m}u\right\|_{\omega^{(\alpha+\beta+m,m)}}, \tag{4.53}$$

where the constant $c\approx 1$ for $N\gg 1$.

Remark 4.5. To have a better understanding of the above approximation results, we compare the GJF with the Legendre approximation to the function

$$u(x)=(1+x)^b g(x),\quad b\in\mathbb{R}^+,\ \ x\in\Lambda, \tag{4.54}$$

where g is analytic in a domain containing Λ. Recall the best L^2-approximation of u by its orthogonal projection $\pi_N^L u$ (see, e.g., [27, Ch. 3])

$$\|\pi_N^L u-u\|\le cN^{-m}\|D^m u\|_{\omega^{(m,m)}}.$$

If b is non-integer, a direct calculation shows that u has a limited regularity: $m<1+2b-\epsilon$ for small $\epsilon>0$, in this usual weighted norm involving derivatives of integer order.

We now consider the GJF approximation (see (4.50)) to u in (4.54). Using the explicit formulas for fractional integral/derivative of $(1+x)^b$ and the Leibniz formula (see [7, Ch. 2]), we find that if $\beta=b$, ${}_{-1}D_x^{\beta+m}u$ is analytic for any $m\in\mathbb{N}_0$, so by (4.50) with $\alpha=0,\beta=b$ and $m=N$, and using (4.26), we have

$$\left\|{}^{-}\pi_N^{(0,-\beta)}u-u\right\|\le\left\|{}^{-}\pi_N^{(0,-\beta)}u-u\right\|_{\omega^{(0,-\beta)}}\le cN^{-(\beta+1/4)}\Big(\frac{e}{2N}\Big)^N\left\|{}_{-1}D_x^{\beta+N}u\right\|_{\omega^{(\beta+N,N)}}.$$

This implies the exponential convergence $O(e^{-cN})$.

Also note that if u is smooth, i.e., $b\in\mathbb{N}$, we can only get a limited convergence rate by choosing a non-integer β. Indeed, a direct calculation by using the Leibniz formula in [7] yields

$${}_{-1}D_x^{\beta+m}u=(1+x)^{b-\beta-m}h(x),$$

where h is analytic. Therefore, $\left\|{}_{-1}D_x^{\beta+m}u\right\|_{\omega^{(\beta+m,m)}}<\infty$, only when $m+2\beta<1+2b-\epsilon$. □

5. Applications to fractional differential equations

It is well known that the underlying solution of an FDE usually exhibits singular behaviors at one or both endpoint(s), even when the given data are smooth. Accordingly, the solution and data are not always in the same types of Sobolev spaces as opposite to differential equations of integer derivatives. Hence, the use of polynomial approximations can only achieve a limited convergence order. In this section, we shall construct Petrov-Galerkin spectral methods using GJFs as basis functions for several prototypical FDEs, and demonstrate the following:

(i) The convergence rate of our approach only depends on the regularity of the data in the usual weighted Sobolev space, regardless of the singular behavior of their solutions. Truly spectral accuracy can be achieved, if the input of a FDE is smooth enough.
(ii) With a suitable choice of the parameters in the GJF basis, the resulting linear systems are usually sparse and sometimes diagonal.

We shall provide ample numerical results to validate the theoretical analysis. We remark that the study of these prototypical FDEs can shed light on the investigation of more complicated FDEs.

5.1. **Fractional initial value problems (FIVPs).** As the first example, we consider the fractional initial value problem of order $s \in (k-1, k)$ with $k \in \mathbb{N}$:

$$ {}_xD_1^s\, u(x) = f(x), \quad x \in \Lambda; \quad u^{(l)}(1) = 0, \quad l = 0, \cdots, k-1, \tag{5.1} $$

where f is continuous on $\bar{\Lambda}$.

The GJF-spectral-Petrov-Galerkin scheme is to find $u_N \in {}^{+}\mathcal{F}_N^{(-s,-s)}(\Lambda)$ (defined in (4.5)) such that

$$ ({}_xD_1^s\, u_N, v_N) = (\mathcal{I}_N f, v_N), \quad \forall\, v_N \in \mathcal{P}_N, \tag{5.2} $$

where $\mathcal{I}_N f$ is the Legendre-Gauss-Lobatto interpolation of f on $(N+1)$ Legendre-Gauss-Lobatto points. Note that

$$ (\mathcal{I}_N f)(x) = \sum_{n=0}^{N} \tilde{f}_n\, P_n(x), \tag{5.3} $$

where P_n is the Legendre polynomial of degree n, and $\{\tilde{f}_q\}$ are the "pseudo-spectral" coefficients computed by the discrete Legendre transform (see, e.g., [27, Ch. 3]). Using the GJF basis, we can write

$$ u_N(x) = \sum_{n=0}^{N} \tilde{u}_n^{(s)}\, {}^{+}J_n^{(-s,-s)}(x) \in {}^{+}\mathcal{F}_N^{(-s,-s)}(\Lambda). \tag{5.4} $$

Taking $v_N = P_l$ in (5.2), we obtain from (3.14) and the orthogonality of Legendre polynomials that

$$ \tilde{u}_n^{(s)} = \frac{n!}{\Gamma(n+s+1)} \tilde{f}_n, \quad 0 \le n \le N. \tag{5.5} $$

Therefore, we obtain the numerical solution u_N by inserting (5.5) into (5.4).

The following error estimate shows the spectral accuracy of this GJF-Petrov-Galerkin scheme.

Theorem 5.1. *Let u and u_N be the solutions of (5.1) and (5.2), respectively. If $f \in C(\bar{\Lambda})$ and $f^{(l)} \in L^2_{\omega^{(l-1,l-1)}}(\Lambda)$ for all $1 \le l \le m$, then we have that for $s \in (k-1,k)$ with $k \in \mathbb{N}$, and $1 \le m \le N+1$,*

$$\|{}_xD_1^s(u-u_N)\| + \|u-u_N\| \le cN^{-m}\|f^{(m)}\|_{\omega^{(m-1,m-1)}}, \tag{5.6}$$

where c is a positive constant independent of u, N, and m.

Proof. Let ${}^{+}\pi_N^{(-s,-s)}u$ be the same as in (4.16) for $0 < s < 1$, and as in (4.37) for $s > 1$, respectively. By (4.17) (with $l = 0$) and (4.37), we have

$$\big({}_xD_1^s({}^{+}\pi_N^{(-s,-s)}u - u), \psi\big) = 0, \quad \forall\, \psi \in \mathcal{P}_N.$$

Then by (5.1),

$$\big(f - {}_xD_1^s\ {}^{+}\pi_N^{(-s,-s)}u, \psi\big) = \big({}_xD_1^s u - {}_xD_1^s\ {}^{+}\pi_N^{(-s,-s)}u, \psi\big) = 0, \quad \forall\, \psi \in \mathcal{P}_N. \tag{5.7}$$

Let $\pi_N f$ be the L^2-orthogonal projection of f upon $\mathcal{P}_N$. We infer from (5.7) that ${}_xD_1^s\ {}^{+}\pi_N^{(-s,-s)}u = \pi_N f$. On the other hand, by (5.2), ${}_xD_1^s\, u_N = \mathcal{I}_N f$. Therefore, we have

$$\big\|{}_xD_1^s({}^{+}\pi_N^{(-s,-s)}u - u_N)\big\| = \|\pi_N f - \mathcal{I}_N f\|. \tag{5.8}$$

Using the triangle inequality leads to

$$\begin{aligned}\|{}_xD_1^s(u-u_N)\| &\le \big\|{}_xD_1^s(u - {}^{+}\pi_N^{(-s,-s)}u)\big\| + \|\pi_N f - \mathcal{I}_N f\| \\ &\le \big\|{}_xD_1^s(u - {}^{+}\pi_N^{(-s,-s)}u)\big\| + \|\pi_N f - f\| + \|f - \mathcal{I}_N f\|.\end{aligned} \tag{5.9}$$

Therefore, it follows from Theorem 4.1 (with $\alpha = -\beta = s$ and $0 < s < 1$), Theorem 4.2 (with $\alpha = -\beta = s$ and $s > 1$), and the Legendre polynomial and interpolation approximation results (see, e.g., [27, Ch. 3]) that

$$\|{}_xD_1^s(u-u_N)\| \le cN^{-m}\big(\|{}_xD_1^{s+m}u\big\|_{\omega^{(m,m)}} + \|f^{(m)}\|_{\omega^{(m-1,m-1)}}\big). \tag{5.10}$$

We deduce from (5.1) that

$$\big\|{}_xD_1^{s+m}u\big\|_{\omega^{(m,m)}} \le c\big\|f^{(m)}\big\|_{\omega^{(m-1,m-1)}}.$$

This leads to the estimate of $\|{}_xD_1^s(u-u_N)\|$.

We now turn to the L^2-estimate. For $s \in \mathbb{R}^+$, ${}_xI_1^s : L^2(\Lambda) \to L^2(\Lambda)$ is a bounded linear operator (see, e.g., [10]). Thus, we have

$$\big\|{}_xI_1^s\,{}_xD_1^s(u-u_N)\big\| \le c\big\|{}_xD_1^s(u-u_N)\big\|. \tag{5.11}$$

We next show that

$$u - u_N = {}_xI_1^s\,{}_xD_1^s(u-u_N). \tag{5.12}$$

As $D^l(u-u_N)(1) = 0$ for $l = 0, \ldots, k-1$, we obtain from (2.8) and (2.11) that

$${}_xD_1^s(u-u_N) = {}_x^CD_1^s(u-u_N) = (-1)^k\,{}_xI_1^{k-s}D^k(u-u_N). \tag{5.13}$$

Using the properties (cf. [7]): ${}_xI_1^s\,{}_xI_1^{k-s} = {}_xI_1^k$ and $(-1)^k\,{}_xI_1^kD^kv = v$, we obtain (5.12) from (5.13) immediately. Thus, by (5.11) and (5.12), we derive the L^2-estimate. □

Remark 5.1. One can also construct a similar GJF-Petrov-Galerkin scheme for the following more general FIVPs of order $s \in (k-1, k)$ with $k \in \mathbb{N}$,

(5.14)
$$\mathcal{L}[u] := {}_xD_1^s u(x) + p_1(x)\ {}_xD_1^{s-1}u(x) + \cdots + p_{k-1}(x)\ {}_xD_1^{s-k+1}u(x) = f(x), \quad x \in \Lambda;$$
$$u^{(l)}(1) = 0, \quad l = 0, \cdots, k-1,$$

where f and $\{p_j\}$ are continuous functions on $\bar{\Lambda}$. We find from (3.12) that $\mathcal{L}[{}^{+}J_n^{(-s,s)}]$ is a combination of products of p_j and polynomials. Hence, one can derive spectrally accurate error estimates as in Theorem 5.1. If $\{p_j\}$ are constants, the corresponding linear system will be sparse; for general $\{p_j\}$, one can use a preconditioned iterative algorithm as in the integer s case by using the problem with suitable constant coefficients as a preconditioner (cf. [27]). □

5.2. **Fractional boundary value problems (FBVPs).** In accordance with usual boundary value problems, it is necessary to classify an FBVP of order ν as even or odd order as follows.

- If $\nu = s + k$ with $s \in (k-1, k)$ and $k \in \mathbb{N}$, we say it is of even order. In this case, $2k$ boundary conditions should be imposed.
- If $\nu = s + k$ with $s \in (k, k+1)$ and $k \in \mathbb{N}$, we say it is odd order. In this case, $2k+1$ boundary conditions should be imposed.

In practice, the boundary conditions can be of integral type or of usual Dirichlet type, which oftentimes lead to different singular behaviors of the solution and should be treated quite differently. In what follows, we first consider FBVPs with integral boundary conditions (BCs), and then discuss Dirichlet boundary conditions.

5.2.1. *FBVPs with integral BCs.* To fix the idea, we consider the fractional boundary value problem of order $\nu \in (1, 2)$:

$$ {}_xD_1^\nu u(x) = f(x), \quad x \in \Lambda; \quad {}_xI_1^\mu u(\pm 1) = 0, \tag{5.15}$$

where $\mu := 2 - \nu \in (0, 1)$, and ${}_xI_1^\mu$ is the fractional integral operator defined in (2.2). Here, $f(x)$ is a given function with regularity to be specified later.

Let $H_0^1(\Lambda) = \{u \in H^1(\Lambda) : u(\pm 1) = 0\}$, and let $H^{-1}(\Lambda)$ be its dual space. Recall the property: ${}_xD_1^\nu = D^2\,{}_xI_1^\mu$ (cf. (2.8)). A weak form of (5.15) is to find $v := {}_xI_1^\mu u \in H_0^1(\Lambda)$ such that

$$(Dv, Dw) = -(f, w), \quad \forall\, w \in H_0^1(\Lambda). \tag{5.16}$$

It is well known that for any $f \in H^{-1}(\Lambda)$, it admits a unique solution $v \in H_0^1(\Lambda)$. Then we can recover u uniquely from $u = {}_xD_1^\mu v$, thanks to (2.9).

As already mentioned, it is important to understand the singular behavior of the solution so as to compass the choice of the parameter that can match the singularity. For this purpose, we act on both sides of (5.15) and impose ${}_xI_1^2$ the boundary conditions, leading to

$$ {}_xI_1^\mu u(x) = {}_xI_1^2 f(x) - \frac{{}_xI_1^2 f(-1)}{2}(1 - x). \tag{5.17}$$

Using the properties (cf. [7]) ${}_xI_1^2 = {}_xI_1^\mu\, {}_xI_1^{2-\mu}$ and ${}_xD_1^\mu(1-x) = (1-x)^{1-\mu}/\Gamma(2-\mu)$, we obtain from (2.9) that

$$u(x) = {}_xD_1^\mu\, {}_xI_1^\mu u(x) = {}_xI_1^{2-\mu} f(x) - \frac{{}_xI_1^2 f(-1)}{2\Gamma(2-\mu)}(1-x)^{1-\mu}. \tag{5.18}$$

Correspondingly, we define the finite-dimensional fractional-polynomial solution space

$$V_N := \big\{\phi = (1-x)^{1-\mu}\psi \,:\, \psi \in \mathcal{P}_{N-1} \ \text{ such that } \ {}_xI_1^{\mu}\phi(-1) = 0\big\}. \tag{5.19}$$

The GJF-Petrov-Galerkin approximation is to find $u_N \in V_N$ such that

$$({}_xD_1^{1-\mu}u_N,\, Dw_N) = (f, w_N), \quad \forall w_N \in \mathcal{P}_N^0 := \mathcal{P}_N \cap H_0^1(\Lambda). \tag{5.20}$$

In terms of error analysis, it is more convenient to formulate (5.20) into an equivalent Galerkin approximation (see (5.25) below). Indeed, note that

$$\mathcal{P}_N = \text{span}\big\{P_n^{(1-\mu,\mu-1)} \,:\, 0 \le n \le N\big\}, \tag{5.21}$$

and by (2.34) with $\rho = \mu, \alpha = 1-\mu$ and $\beta = \mu - 1$,

(5.22)

$${}_xI_1^{\mu}\,{}^{+}J_n^{(\mu-1,\mu-1)}(x) = \frac{\Gamma(n+2-\mu)}{(n+1)!}\,{}^{+}J_n^{(-1,-1)}(x) = \frac{\Gamma(n+2-\mu)}{n!}\int_x^1 P_n(y)dy,$$

where we used the formula derived from integrating the Sturm-Liouville equation of Legendre polynomials and using (3.16),

(5.23)

$${}_xI_1^1P_n(x) = \int_x^1 P_n(y)dy = \frac{1}{2n}(1-x^2)P_{n-1}^{(1,1)}(x) = \frac{1}{n+1}\,{}^{+}J_n^{(-1,-1)}(x), \ \ n \ge 1.$$

Since for $n \ge 1$, ${}_xI_1^{\mu}\,{}^{+}J_n^{(\mu-1,\mu-1)}(\pm 1) = 0$, we have

(5.24)

$$V_N = \text{span}\big\{{}^{+}J_n^{(\mu-1,\mu-1)} \,:\, 1 \le n \le N-1\big\}; \quad \mathcal{P}_N^0 = \text{span}\big\{{}_xI_1^1P_n \,:\, 1 \le n \le N-1\big\}.$$

Thus, we infer from (5.22) that the operator ${}_xI_1^{\mu}$ is an isomorphism between V_N and $\mathcal{P}_N^0$. Then we can equivalently formulate (5.20) as follows. Find $v_N := {}_xI_1^{\mu}u_N \in \mathcal{P}_N^0$ such that

$$(Dv_N,\, Dw_N) = -(f, w_N), \quad \forall w_N \in \mathcal{P}_N^0. \tag{5.25}$$

It admits a unique solution as with (5.16). In fact, this formulation facilitates the error analysis, which can be accomplished by a standard argument as follows.

Theorem 5.2. *Let u and u_N be the solution of* (5.15) *and* (5.25)*, respectively. If ${}_xI_1^{\mu}u \in H_0^1(\Lambda)$ and $(1-x^2)^{(m-1)/2}\,{}_xD_1^{m-\mu}u \in L^2(\Lambda)$ with $m \in \mathbb{N}$, then we have*

$$\|{}_xD_1^{1-\mu}(u-u_N)\| \le cN^{1-m}\|{}_xD_1^{m-\mu}u\|_{\omega^{(m-1,m-1)}}. \tag{5.26}$$

In particular, if $f^{(m-2)} \in L^2_{\omega^{(m-1,m-1)}}(\Lambda)$ with $m \ge 2$, we have

$$\|{}_xD_1^{1-\mu}(u-u_N)\| \le cN^{1-m}\|f^{(m-2)}\|_{\omega^{(m-1,m-1)}}. \tag{5.27}$$

Here, c is a positive constant independent of N and u.

Proof. Using a standard argument for error analysis of Galerkin approximation, we find from (5.16) and (5.25) that

$$\|D(v-v_N)\| = \inf_{v_N^* \in \mathcal{P}_N^0}\|D(v-v_N^*)\|. \tag{5.28}$$

Let $\pi_N^{1,0}$ be the usual H_0^1-orthogonal projection upon $\mathcal{P}_N^0$, and recall the approximation result (see, e.g., [27, Ch. 3]),

$$\|D(v-\pi_N^{1,0}v)\| \le cN^{1-m}\|D^m v\|_{\omega^{(m-1,m-1)}}. \tag{5.29}$$

Recall that $v = {}_xI_1^\mu u$ and $v_N = {}_xI_1^\mu u_N$, so we take $v_N^* = \pi_N^{1,0} v$ in (5.28) and obtain the desired estimate (5.26) from (5.29).

The estimate (5.27) follows immediately from (5.15) and (5.26) by noting that $D^{m-2} f = {}_xD_1^{m-\mu} u$. □

Remark 5.2. By using the duality argument, one can derive an optimal L^2-error estimate for $v - v_N$,

$$\|v - v_N\| \le cN^{-m} \|D^m v\|_{\omega^{(m-1,m-1)}},$$

which implies

$$\|{}_xI_1^\mu (u - u_N)\| \le cN^{-m} \|{}_xD_1^{m-\mu} u\|_{\omega^{(m-1,m-1)}}.$$

However, due to the lack of regularity for (5.15), we are unable to use the duality argument to get an improved estimate for $\|u - u_N\|$. □

Now, we briefly describe the implementation of the scheme (5.20). Setting

$$u_N(x) = \sum_{n=1}^{N-1} \hat{u}_n {}^+J_n^{(\mu-1,\mu-1)}(x), \quad f_j = (f, I_+^1 P_j), \ \ 1 \le j \le N-1,$$

we find from (5.22) and the orthogonality of Legendre polynomials that

$$\big({}_xD_1^{1-\mu} {}^+J_n^{(\mu-1,\mu-1)},\, D_x I_1^1 P_j\big) = \frac{\Gamma(n+2-\mu)}{n!} \frac{2n+1}{2} \delta_{jn}. \tag{5.30}$$

Then we obtain from (5.20) that

$$\hat{u}_n = \frac{2(n!) f_n}{(2n+1)\Gamma(n+2-\mu)}, \quad 1 \le n \le N-1. \tag{5.31}$$

We see that using the GJFs as basis functions, the matrix of the linear system is diagonal.

Remark 5.3. The above approach can be applied to higher-order FBVPs. For example, we consider the FBVP of "odd" order: for $\nu = 3 - \mu$ with $\mu \in (0,1)$,

$${}_xD_1^\nu u(x) = f(x), \ \ x \in \Lambda; \quad {}_xI_1^\mu u(\pm 1) = ({}_xI_1^\mu u)'(1) = 0. \tag{5.32}$$

To avoid repetition, we just outline the numerical scheme and implementation. Define the solution and test function spaces

$$\begin{aligned} V_N &:= \big\{\phi = (1-x)^{2-\mu}\psi \ : \psi \in \mathcal{P}_{N-2} \ \text{ such that } \ {}_xI_1^\mu \phi(-1) = 0\big\}, \\ V_N^* &:= \{\psi \in \mathcal{P}_N \ : \ \psi(\pm 1) = \psi'(-1) = 0\}. \end{aligned} \tag{5.33}$$

The GJF-Petrov-Galerkin scheme is to find $u_N \in V_N$ such that

$$({}_xD_1^{2-\mu} u_N, Dw_N) = (f, w_N), \quad \forall w_N \in V_N^*. \tag{5.34}$$

Using (2.34) with $\rho = \mu, \alpha = 2-\mu$ and $\beta = \mu - 1$, we obtain from (2.25) that

$$\begin{aligned} &{}_xI_1^\mu \ {}^+J_n^{(\mu-2,\mu-1)}(x) = \frac{\Gamma(n+3-\mu)}{(n+2)!} {}^+J_n^{(-2,-1)}(x); \\ &{}_xI_1^\mu \ {}^+J_n^{(\mu-2,\mu-1)}(-1) = 0, \ \ n \ge 1. \end{aligned} \tag{5.35}$$

Hence, we have

$$\begin{aligned} V_N &= \text{span}\big\{{}^+J_n^{(\mu-2,\mu-1)} \ : \ 1 \le n \le N-2\big\}, \\ V_N^* &= \text{span}\big\{{}^-J_n^{(-1,-2)} \ : \ 1 \le n \le N-2\big\}. \end{aligned} \tag{5.36}$$

By (2.5),

$$
\begin{aligned}
&{}_xD_1^{2-\mu}\ {}^{+}J_n^{(\mu-2,\mu-1)}(x) = \frac{\Gamma(n+3-\mu)}{n!}P_n^{(0,1)}(x),\\
&D\ {}^{-}J_m^{(-1,-2)}(x) = (m+2)(1+x)P_m^{(0,1)}(x),
\end{aligned}
\tag{5.37}
$$

so by the orthogonality of the Jacobi polynomials $\{P_n^{(0,1)}\}$, the matrix of the system (5.34) is diagonal. □

5.2.2. *FBVPs with Dirichlet boundary conditions.* Now, we turn to a more complicated case and consider the fractional boundary value problem of even order $\nu = s + k$ with $s \in (k-1, k)$ and $k \in \mathbb{N}$:

$$
{}_xD_1^{\nu}\, u(x) = f(x),\ \ x \in \Lambda; \quad u^{(l)}(\pm 1) = 0,\ \ l = 0, 1, \ldots, k-1,
\tag{5.38}
$$

where $f(x)$ is a given function with regularity to be specified later.

We introduce the solution and test function spaces,

$$
\begin{aligned}
U &:= \big\{u \in L^2_{\omega^{(-s,-k)}}(\Lambda)\ :\ {}_xD_1^s\, u \in L^2_{\omega^{(0,s-k)}}(\Lambda)\big\},\\
V &:= \big\{v \in L^2_{\omega^{(-k,-s)}}(\Lambda)\ :\ D^k v \in L^2_{\omega^{(0,k-s)}}(\Lambda)\big\},
\end{aligned}
\tag{5.39}
$$

equipped with the norms

$$
\begin{aligned}
\|u\|_U &= \big(\|u\|^2_{\omega^{(-s,-k)}} + \|{}_xD_1^s u\|^2_{\omega^{(0,s-k)}}\big)^{1/2},\\
\|v\|_V &= \big(\|v\|^2_{\omega^{(-k,-s)}} + \|D^k v\|^2_{\omega^{(0,k-s)}}\big)^{1/2}.
\end{aligned}
\tag{5.40}
$$

For $u \in U$ and $v \in V$, we write

$$
\begin{aligned}
u(x) &= \sum_{n=k}^{\infty} \hat{u}_n\, {}^{+}J_n^{(-s,-k)}(x) = (1-x)^s(1+x)^k \sum_{n=k}^{\infty} \tilde{u}_n P_{n-k}^{(s,k)}(x),\\
v(x) &= \sum_{n=k}^{\infty} \hat{v}_n\, {}^{-}J_n^{(-k,-s)}(x) = (1-x)^k(1+x)^s \sum_{n=k}^{\infty} \tilde{v}_n P_{n-k}^{(k,s)}(x),
\end{aligned}
\tag{5.41}
$$

where by (3.5), $\tilde{u}_n = 2^{-k} d_n^{k,s} \hat{u}_n$ and $\tilde{v}_n = (-1)^k 2^{-k} d_n^{k,s} \hat{v}_n$.

With the above setup, we can build in the homogenous boundary conditions and also perform fractional integration by parts (cf. Lemma 2.2). Hence, a weak form of (5.38) is to find $u \in U$ such that

$$
a(u, v) := ({}_xD_1^s u,\, D^k v) = (f, v), \quad \forall\, v \in V.
\tag{5.42}
$$

Let ${}^{+}\mathcal{F}_N^{(-s,-k)}(\Lambda)$ and ${}^{-}\mathcal{F}_N^{(-k,-s)}(\Lambda)$ be the finite-dimensional spaces as defined in the previous section. Then the GJF-Petrov-Galerkin scheme for (5.42) is to find $u_N \in {}^{+}\mathcal{F}_N^{(-s,-k)}(\Lambda)$ such that

$$
a(u_N, v_N) = ({}_xD_1^s u_N,\, D^k v_N) = (f, v_N), \quad \forall\, v_N \in {}^{-}\mathcal{F}_N^{(-k,-s)}(\Lambda).
\tag{5.43}
$$

We next show the unique solvability of (5.42)-(5.43) by verifying the Babuška-Brezzi inf-sup condition of the involved bilinear form. For this purpose, we first show the following equivalence of the norms.

Lemma 5.1. *Let $s \in (k-1, k)$ and $k \in \mathbb{N}$, and let U, V be the space defined in* (5.39) *and* (5.40)*, respectively. Then we have*

$$
\begin{aligned}
C_{1,s}\|u\|_U \le \|{}_xD_1^s u\|_{\omega^{(0,s-k)}} \le \|u\|_U, \quad \forall u \in U,\\
C_{2,s}\|v\|_V \le \|D^k v\|_{\omega^{(0,k-s)}} \le \|v\|_V, \quad \forall v \in V,
\end{aligned}
\tag{5.44}
$$

where

(5.45)
$$C_{1,s} = \left(1 + \frac{k!}{\Gamma(k+s+1)\Gamma(s+1)}\right)^{-1/2}, \quad C_{2,s} = \left(1 + \frac{\Gamma(s+1)}{k!\Gamma(k+s+1)}\right)^{-1/2}.$$

Proof. Given the expansion in (5.41), we derive from (3.11) and (3.17) that

$$\|u\|^2_{\omega^{(-s,-k)}} = \sum_{n=k}^{\infty} \gamma_n^{(s,-k)} \big|\hat{u}_n\big|^2, \quad \big\|{}_xD_1^s u\big\|^2_{\omega^{(0,s-k)}} = \sum_{n=k}^{\infty} h_{n,0}^{(s,-k)} \big|\hat{u}_n\big|^2, \tag{5.46}$$

where by (3.18),

$$h_{n,0}^{(s,-k)} = \frac{\Gamma^2(n+s+1)}{(n!)^2} \gamma_n^{(0,s-k)}. \tag{5.47}$$

Therefore,

$$\|u\|^2_{\omega^{(-s,-k)}} = \sum_{n=k}^{\infty} \frac{\gamma_n^{(s,-k)}}{h_{n,0}^{(s,-k)}} h_{n,0}^{(s,-k)} \big|\hat{u}_n\big|^2 \le \frac{\gamma_k^{(s,-k)}}{h_{k,0}^{(s,-k)}} \big\|{}_xD_1^s u\big\|^2_{\omega^{(0,s-k)}},$$

so by (2.30), (5.40), and (5.47),

$$\|u\|^2_U \le \left(1 + \frac{\gamma_k^{(s,-k)}}{h_{k,0}^{(s,-k)}}\right) \big\|{}_xD_1^s u\big\|^2_{\omega^{(0,s-k)}} = \frac{1}{C_{1,s}^2} \big\|{}_xD_1^s u\big\|^2_{\omega^{(0,s-k)}}.$$

This yields the first equivalence relation in (5.44).

Next, we find from (2.7) and (3.13) that

$$D^k\big\{{}^{-}J_n^{(-k,-s)}(x)\big\} = \frac{\Gamma(n+s+1)}{\Gamma(n+s-k+1)} {}^{-}J_n^{(0,k-s)}(x), \tag{5.48}$$

so we have from the orthogonality (3.10)-(3.11) and (5.41) that

$$\|v\|^2_{\omega^{(-k,-s)}} = \sum_{n=k}^{\infty} \big|\hat{v}_n\big|^2 \gamma_n^{(s,-k)}; \quad \big\|D^k v\big\|^2_{\omega^{(0,k-s)}} = \sum_{n=k}^{\infty} q_n^{(s,k)} \big|\hat{v}_n\big|^2, \tag{5.49}$$

where

$$q_n^{(s,k)} := \frac{\Gamma^2(n+s+1)}{\Gamma^2(n+s-k+1)} \gamma_n^{(0,s-k)}. \tag{5.50}$$

Working out the constants leads to

$$\|v\|^2_{\omega^{(-k,-s)}} \le \frac{\gamma_k^{(s,-k)}}{q_k^{(s,k)}} \big\|D^k v\big\|^2_{\omega^{(0,k-s)}} \le \frac{\Gamma(s+1)}{k!\Gamma(k+s+1)} \big\|D^k v\big\|^2_{\omega^{(0,k-s)}}. \tag{5.51}$$

Then by (5.40), the second equivalence follows immediately. □

With the aid of Lemma 5.1, we can show the well-posedness of the weak form (5.42) and the Petrov-Galerkin scheme (5.43).

Theorem 5.3. *Let $f \in L^2_{\omega^{(k,s)}}(\Lambda)$. Then the problem* (5.42) *admits a unique solution $u \in U$, and the scheme* (5.43) *admits a unique solution $u_N \in {}^{+}\mathcal{F}_N^{(-s,-k)}(\Lambda)$.*

Proof. It is clear that we have the continuity of the bilinear form on $U \times V$:

$$|a(u,v)| \le \|u\|_U \|v\|_V, \quad \forall\, u \in U, \ \ \forall\, v \in V. \tag{5.52}$$

The main task is to verify the inf-sup condition; that is, for any $0 \neq u \in U$,

$$\sup_{0 \neq v \in V} \frac{|a(u,v)|}{\|u\|_U \|v\|_V} \ge \eta := C_{1,s} C_{2,s}, \tag{5.53}$$

where $C_{1,s}$ and $C_{2,s}$ are given in (5.45). For this purpose, we construct $v_* \in V$ from the expansion of $u \in U$ in (5.41):

$$v_*(x) := \sum_{n=k}^{\infty} \hat{v}_n^* \, {}^{-}J_n^{(-k,-s)}(x) \quad \text{with} \quad \hat{v}_n^* = \frac{\Gamma(n+s-k+1)}{n!} \hat{u}_n. \tag{5.54}$$

By construction, one verifies by using the orthogonality (2.29), (5.46) and (5.49) that

$$a(u, v_*) = \big\|{}_x D_1^s u\big\|^2_{\omega^{(0,s-k)}} = \big\|D^k v_*\big\|^2_{\omega^{(0,k-s)}}. \tag{5.55}$$

Thus, using Lemma 5.1, we infer that for any $0 \neq u \in U$, there exists $0 \neq v_* \in V$ such that

$$a(u, v_*) = \big\|{}_x D_1^s u\big\|_{\omega^{(0,s-k)}} \big\|D^k v_*\big\|_{\omega^{(0,k-s)}} \ge C_{1,s} C_{2,s} \|u\|_U \|v_*\|_V. \tag{5.56}$$

This implies (5.53).

It remains to verify the "transposed" inf-sup condition

$$\sup_{0 \neq u \in U} |a(u,v)| > 0, \quad \forall\, 0 \neq v \in V. \tag{5.57}$$

It can be shown by a converse process. In fact, assuming that $0 \neq v_* \in V$ is an arbitrary function, we construct

$$u(x) = \sum_{n=k}^{\infty} \hat{u}_n \, {}^{+}J_n^{(-s,-k)}(x) \quad \text{with} \quad \hat{u}_n = \frac{n!}{\Gamma(n+s-k+1)} \hat{v}_n^*.$$

Then we can derive (5.57) using (5.55).

Finally, if $f \in L^2_{\omega^{(k,s)}}(\Lambda)$, we obtain from the Cauchy-Schwarz inequality that

$$|(f,v)| \le \|f\|_{\omega^{(k,s)}} \|v\|_{\omega^{(-k,-s)}} \le \|f\|_{\omega^{(k,s)}} \|v\|_V.$$

Therefore, we claim from the Babuška-Brezzi theorem (cf. [4]) that the problem (5.2) has a unique solution.

Note that the inf-sup condition (5.53) is also valid for the discrete problem (5.43), which therefore admits a unique solution. □

With the help of the above results, we can follow a standard argument to carry out the error analysis.

Theorem 5.4. *Let $s \in (k-1, k)$ with $k \in \mathbb{N}$, and let u and u_N be the solutions of* (5.42) *and* (5.43)*, respectively. If $u \in U \cap {}^{+}\mathcal{B}^m_{s,-k}(\Lambda)$ with $0 \le m \le N$, then we have the error estimates:*

$$\|u - u_N\|_U \le c N^{-m} \big\|{}_x D_1^{s+m} u\big\|_{\omega^{(m,s-k+m)}}. \tag{5.58}$$

In particular, if $f^{(m-k)} \in L^2_{\omega^{(m,s-k+m)}}(\Lambda)$ for $m \ge k$, we have

$$\|u - u_N\|_U \le c N^{-m} \big\|f^{(m-k)}\big\|_{\omega^{(m,s-k+m)}}. \tag{5.59}$$

Here, c is a positive constant independent u, N and m.

Proof. Thanks to the inf-sup condition derived in the proof of the previous theorem, we have

$$\|u-u_N\|_U \le (1+\eta^{-1})\|u-\phi\|_U, \quad \forall\, \phi \in {}^{+}\mathcal{F}_N^{(-s,-k)}(\Lambda), \tag{5.60}$$

where η is the inf-sup constant in (5.53). Let ${}^{+}\pi_N^{(-s,-k)}$ be the orthogonal projection operator as defined in (4.15)-(4.16). Taking $\phi = {}^{+}\pi_N^{(-s,-k)}u$ in (5.60), we obtain from Theorem 4.1 and Lemma 5.1 that

$$\begin{aligned}\|u-u_N\|_U &\le (1+\eta^{-1})\|u-{}^{+}\pi_N^{(-s,-k)}u\|_U\\ &\le (1+\eta^{-1})(C_{1,s})^{-1}\big\|{}_xD_1^s(u-{}^{+}\pi_N^{(-s,-k)}u)\big\|_{\omega^{(0,s-k)}}\\ &\le cN^{-m}\big\|{}_xD_1^{s+m}u\big\|_{\omega^{(m,s-k+m)}}.\end{aligned} \tag{5.61}$$

This yields (5.58).

From the original equation (5.38), we obtain ${}_xD_1^{\nu}u = {}_xD_1^{s+k}u = f$, so (5.59) follows from (5.58) immediately. □

Remark 5.4. By using a similar procedure as above, we can also construct a spectral Petrov-Galerkin method for the odd order FBVP of order $\nu = s+k$ and $s \in (k, k+1)$ with $k \in \mathbb{N}$,

$${}_xD_1^{\nu}u(x) = f(x), \ \ x \in \Lambda, \quad u^{(l)}(\pm 1) = 0, \ \ l = 0, 1, \ldots, k-1, \ \ u^{(k)}(1) = 0, \tag{5.62}$$

and establish an error estimate as in Theorem 5.4. □

5.3. **Numerical results.** In what follows, we provide numerical results to illustrate the accuracy of the proposed GJF-Petrov-Galerkin schemes and to validate the theoretical results. We consider two typical situations for both FIVP and FBVP:

(i) the source term $f(x)$ is smooth, but the solution $u(x)$ is singular; and

(ii) the solution $u(x)$ is smooth, but the source term $f(x)$ is singular.

We measure the numerical errors by the discrete version of $\|{}_xD_1^s(u-u_N)\|$ (called "fractional norm" for simplicity) and discrete L^2-norm.

5.3.1. *Fractional initial value problems.* (i) We consider the FIVP (5.1) with $f(x) = 1 + x + \cos x$, whose solution has a singular behavior $O((1-x)^s)$. In this case, it is hard to find a closed form solution of (5.1), so we use very fine grids to compute a reference "exact" solution. (ii) We take the exact solution of (5.1) to be $u(x) = (1-\exp(1-x))(1-x^3)$ and note that the source term has singularity at $x = 1$.

As predicted by Theorem 5.1, the errors of the former are expected to decay exponentially fast, despite the singular behavior of the solution near $x = 1$. Indeed, we observe such a decay from Figure 5.1 (left). In the second case, following the argument in Remark 4.5, we find from $u = (1-\exp(1-x))(1-x^3) \sim (1-x)^2 g(x)$ that

$${}_xD_1^{s+m}u(x) = O((1-x)^{2-s-m}), \quad x \to 1,$$

which implies $\|{}_xD_1^{s+m}u\|_{\omega^{(m,m)}} < +\infty$, if $m < 5-2s$. In Figure 5.1 (right), we depict the errors against $\log_{10} N$ for $s = 1.4$ and $s = 1.9$. Indeed, the slopes of the lines are approximately -2 and -1, which agree well with the theoretical result.

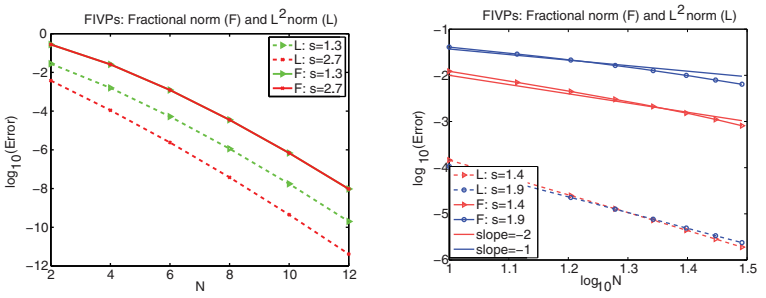

FIGURE 5.1. Examples of FIVPs. Left: $f(x) = 1 + x + \cos x$. Right: $u(x) = (1 - \exp(1-x))(1-x^3)$.

We also observe from Figure 5.1 (left) that the L^2-errors for $s = 1.3, 2.7$ are nearly the same, owing to the fact that the convergence of the scheme is completely determined by regularity of the source term $f(x)$ in the usual Sobolev space (see Theorem 5.1).

5.3.2. *Fractional boundary value problems with integral boundary conditions.* We now consider the FBVP (5.15) with $\mu \in (0, 2)$ and

(i) $\nu = 3 - \mu$ and smooth source term $f(x) = \sin x$, and

(ii) $\nu = 2 - \mu$ and smooth exact solution $u(x) = (1-x)^3 - 6(1-x)^2/(3+\mu)$.

As shown in Theorem 5.2, we observe an exponential convergence for case (i) (see Figure 5.2 (left)) and an algebraic convergence for case (ii) (see Figure 5.2 (right)). As before, we can estimate the rate of algebraic decay for case (ii) by a direct calculation of the norms in the upper bounds of the estimates in Theorem 5.2, which again agrees with the numerical results in Figure 5.2 (right).

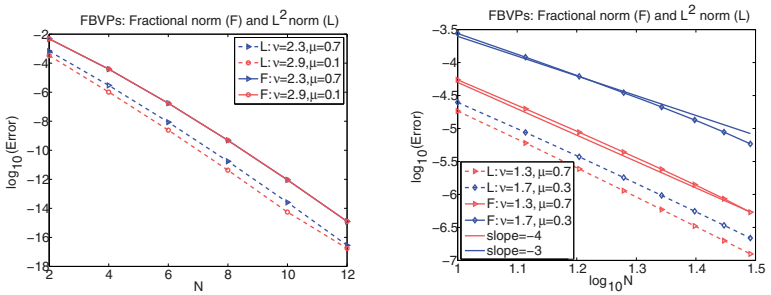

FIGURE 5.2. FBVPs with integral boundary conditions. Left: $f(x) = \sin x$. Right: $u(x) = (1-x)^3 - 6(1-x)^2/(3+\mu)$.

5.3.3. *Fractional boundary value problems with homogeneous boundary conditions.* Next, we provide numerical results for the FBVP (5.38). Once again, we consider two cases:

(i) $\nu = 2 + s$ and smooth source term $f(x) = xe^x$, and

(ii) $\nu = 1 + s$ and smooth solution $u(x) = (1-x)\sin(\pi x)$.

Like the previous cases, the error plots in Figure 5.3 show the convergence behaviours in accordance with the estimates in Theorem 5.4.

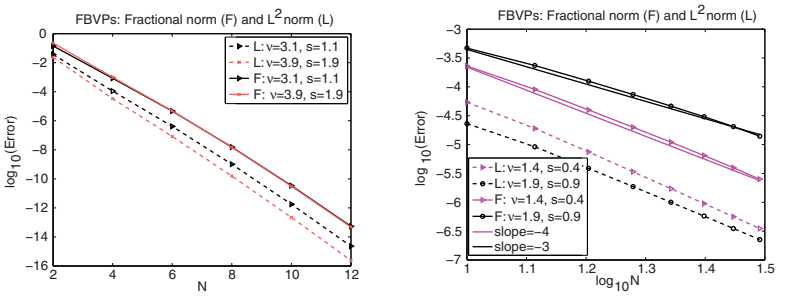

FIGURE 5.3. FBVPs with homogeneous boundary conditions. Left: $f(x) = xe^x$. Right: $u(x) = (1-x)\sin(\pi x)$.

6. Extension to Caputo fractional derivatives

In this section, we extend the GJF approximation in Sobolev spaces involving Riemann-Liouville fractional derivatives to Caputo fractional derivatives. We conclude the paper with some remarks.

6.1. **Important formulas.** It is seen that the formulas in Lemma 2.5 and Theorem 3.1 are exceedingly important in the analysis and spectral algorithms for FDEs involving Riemann-Liouville derivatives. Remarkably, similar formulas are also available for the Caputo fractional derivatives. Like Lemma 2.5, we have the following formulas.

Lemma 6.1. *Let $s \in [k-1, k)$ with $k \in \mathbb{N}, n \in \mathbb{N}_0$, and $x \in \Lambda$.*

- *For $\alpha > -1$ and $\beta \in \mathbb{R}$,*

$$\begin{aligned} &{}_x^C D_1^s\big\{(1-x)^{\alpha+k} P_n^{(\alpha+k,\beta-k)}(x)\big\} \\ &\quad = \frac{\Gamma(n+\alpha+k+1)}{\Gamma(n+\alpha+k-s+1)}(1-x)^{\alpha+k-s} P_n^{(\alpha+k-s,\beta-k+s)}(x). \end{aligned} \tag{6.1}$$

- *For $\alpha \in \mathbb{R}$ and $\beta > -1$,*

$$\begin{aligned} &{}_{-1}^C D_x^s\big\{(1+x)^{\beta+k} P_n^{(\alpha-k,\beta+k)}(x)\big\} \\ &\quad = \frac{\Gamma(n+\beta+k+1)}{\Gamma(n+\beta+k-s+1)}(1+x)^{\beta+k-s} P_n^{(\alpha-k+s,\beta+k-s)}(x). \end{aligned} \tag{6.2}$$

Proof. Let us first derive (6.1). In view of ${}_xD_1^k = (-1)^k D^k$ with $k \in \mathbb{N}$ (cf. (2.7)), we obtain from (2.36) that

$$D^k\big\{(1-x)^{\alpha+k} P_n^{(\alpha+k,\beta-k)}(x)\big\} = (-1)^k \frac{\Gamma(n+\alpha+k+1)}{\Gamma(n+\alpha+1)}(1-x)^{\alpha} P_n^{(\alpha,\beta)}(x). \tag{6.3}$$

By Definition 2.1, we have ${}_x^C D_1^s v = (-1)^k {}_xI_1^{k-s}(D^k v)$, so using (2.34) with $\rho = k-s$ and (6.3) leads to

$$\begin{aligned} &{}_x^C D_1^s\big\{(1-x)^{\alpha+k} P_n^{(\alpha+k,\beta-k)}(x)\big\} \\ &\quad = \frac{\Gamma(n+\alpha+k+1)}{\Gamma(n+\alpha+1)} {}_xI_1^{k-s}\big\{(1-x)^{\alpha} P_n^{(\alpha,\beta)}(x)\big\} \\ &\quad = \frac{\Gamma(n+\alpha+k+1)}{\Gamma(n+\alpha+k-s+1)}(1-x)^{\alpha+k-s} P_n^{(\alpha+k-s,\beta-k+s)}(x). \end{aligned}$$

This yields (6.1). The formula (6.2) can be derived similarly. □

The counterpart of Theorem 3.1 takes a slightly different form in the range of parameters, which is a direct consequence of Lemma 6.1.

Theorem 6.1. *Let $s \in [k-1, k)$ with $k \in \mathbb{N}$, $n \in \mathbb{N}_0$ and $x \in \Lambda$.*

- *For $\alpha > k-1$ and $\beta \in \mathbb{R}$,*

$$ {}_x^C D_1^s \big\{ {}^+J_n^{(-\alpha,\beta)}(x) \big\} = \frac{\Gamma(n+\alpha+1)}{\Gamma(n+\alpha-s+1)} {}^+J_n^{(-\alpha+s,\beta+s)}(x). \tag{6.4} $$

- *For $\alpha \in \mathbb{R}$ and $\beta > k-1$,*

$$ {}_{-1}^C D_x^s \big\{ {}^-J_n^{(\alpha,-\beta)}(x) \big\} = \frac{\Gamma(n+\beta+1)}{\Gamma(n+\beta-s+1)} {}^-J_n^{(\alpha+s,-\beta+s)}(x). \tag{6.5} $$

Proof. With $(\alpha-k, \beta+k)$ in place of (α, β) in (6.1), we obtain (6.4) immediately from the definition (3.1). The rule (6.5) can be obtained in the same fashion.

Alternatively, note that

$$ D^l {}^+J_n^{(-\alpha,\beta)}(x) = D^l((1-x)^\alpha P_n^{(\alpha,\beta)}(x)) = (1-x)^{\alpha-l}\phi(x), \tag{6.6} $$

for some $\phi \in \mathcal{P}_n$, so $D^l {}^+J_n^{(-\alpha,\beta)}(1) = 0$ for $l = 0, \ldots, k-1$. Then by (2.11), we have ${}_x^C D_1^s {}^+J_n^{(-\alpha,\beta)}(x) = {}_x D_1^s {}^+J_n^{(-\alpha,\beta)}(x)$. Therefore, (6.4) follows from (3.12) straightforwardly. □

Taking $s = \alpha$ in (6.4) leads to that for $\alpha > 0$ and $\beta \in \mathbb{R}$,

$$ {}_x^C D_1^\alpha \big\{ {}^+J_n^{(-\alpha,\beta)}(x) \big\} = \frac{\Gamma(n+\alpha+1)}{n!} P_n^{(0,\alpha+\beta)}(x). \tag{6.7} $$

Similarly, we derive from (6.5) an important formula; that is, for $\alpha \in \mathbb{R}$ and real $\beta > 0$,

$$ {}_{-1}^C D_x^\beta \big\{ {}^-J_n^{(\alpha,-\beta)}(x) \big\} = \frac{\Gamma(n+\beta+1)}{n!} P_n^{(\alpha+\beta,0)}(x). \tag{6.8} $$

When $\alpha \in \mathbb{N}$, the above formulas are identical to (3.12)-(3.13), respectively.

6.2. **Approximation results.** The argument to derive the GJF approximation results in Subsection 4.1 essentially relies on the orthogonality of Riemann-Liouville fractional derivatives of GJFs. Notably, we have very similar orthogonal properties in the Caputo case.

Using (3.16) and (6.7)-(6.8), the orthogonality (3.17) and (3.19) takes the following form.

- For $\alpha > 0$ and $\alpha + \beta > -1$,

$$ \int_{-1}^{1} D^l \, {}_x^C D_1^\alpha \, {}^+J_n^{(-\alpha,\beta)}(x) \; D^l \, {}_x^C D_1^\alpha \, {}^+J_{n'}^{(-\alpha,\beta)}(x) \, \omega^{(l,\alpha+\beta+l)}(x) \, dx = h_{n,l}^{(\alpha,\beta)} \delta_{nn'}. \tag{6.9} $$

- For $\alpha + \beta > -1$ and $\beta > 0$,

$$ \int_{-1}^{1} D^l \, {}_{-1}^C D_x^\beta \, {}^-J_n^{(\alpha,-\beta)}(x) \; D^l \, {}_{-1}^C D_x^\beta \, {}^-J_{n'}^{(\alpha,-\beta)}(x) \, \omega^{(\alpha+\beta+l,l)}(x) \, dx = h_{n,l}^{(\beta,\alpha)} \delta_{nn'}. \tag{6.10} $$

Here, $l \in \mathbb{N}_0$ and $h_{n,l}^{(\alpha,\beta)}$ is defined in (3.18).

In view of the above orthogonality, we modify the definition of the space in (4.18) as

$$
{}_{+}^{C}\mathcal{B}^m_{\alpha,\beta}(\Lambda) := \big\{u \in L^2_{\omega^{(-\alpha,\beta)}}(\Lambda) \,:\, D^l\, {}_x^C D_1^\alpha u \in L^2_{\omega^{(l,\alpha+\beta+l)}}(\Lambda),\ \ l = 0, 1, \cdots, m\big\}, \tag{6.11}
$$

for $m \in \mathbb{N}_0$. Similarly, we can define ${}_{-}^{C}\mathcal{B}^m_{\alpha,\beta}(\Lambda)$. Let ${}^{+}\Upsilon_i^{\alpha,\beta}, i = 1, 2, 3$, be the same as in (4.4). Then (4.19) holds for $(\alpha, \beta) \in {}^{+}\Upsilon_1^{\alpha,\beta} \cup {}^{+}\Upsilon_2^{\alpha,\beta}$ and $l \in \mathbb{N}_0$, with $D^l\, {}_x^C D_1^\alpha$ in place of ${}_xD_1^{\alpha+l}$, namely,

$$
\big\|D^l\, {}_x^C D_1^\alpha\, u\big\|^2_{\omega^{(l,\alpha+\beta+l)}} = \sum_{n=\tilde{l}}^{\infty} h_{n,\tilde{l}}^{(\alpha,\beta)} \big|\hat{u}_n^{(\alpha,\beta)}\big|^2. \tag{6.12}
$$

Thanks to (6.9)-(6.10), we can extend the results in Subsection 4.1 to the Caputo fractional derivatives by using the same argument.

Theorem 6.2. *The approximation results in Theorems* 4.1 and 4.2 *hold for the Caputo derivatives with* $D^k\, {}_x^C D_1^\alpha$ $(k = 0, l, m)$ *and* ${}_{+}^{C}\mathcal{B}^m_{\alpha,\beta}(\Lambda)$ *in place of* ${}_xD_1^{\alpha+k}$ $(k = 0, l, m)$ *and* ${}^{+}\mathcal{B}^m_{\alpha,\beta}(\Lambda)$, *respectively. Likewise, the results in Theorems* 4.3 and 4.4 *can be extended to the left-hand side of the Caputo derivatives.*

Proof. Note that in the Riemann-Liouville case, we have ${}_xD_1^{\alpha+k} = (-1)^k D^k\, {}_xD_1^\alpha$ and ${}_{-1}D_x^{\alpha+k} = D^k\, {}_{-1}D_x^\alpha$ for $\alpha \in \mathbb{R}^+$ and $k \in \mathbb{N}$, but this rule does not hold for the Caputo fractional derivatives. Leaving the derivative operator D^k as it stands, we can use the orthogonality (6.9)-(6.10) (to replace (3.17) and (3.19)), and follow the same lines as in the proofs of Theorems 4.1 and 4.2 to derive the desired approximation results. □

6.3. **Discussions and concluding remarks.** We considered in this paper spectral approximation of FDEs by introducing a class of priorly defined GJFs.

Our main contributions are twofold:

- We introduce a new class of GJFs, which extend the range of definition of poly-fractonomials [32] so that high-order fractional derivatives can be treated, and their relations with fractional derivatives, and their approximation properties can be studied.
- We constructed Petrov-Galerkin spectral methods for a class of prototypical FDEs, including arbitrarily high-order FIVPs and FBVPs which have not been numerically studied before, which led to sparse matrices. We derived error estimates with convergence rate only depending on the smoothness of data. In particular, if the data are analytic, we obtain exponential convergence, despite the fact that the solution is singular.

The results presented in this paper indicate that, at least for the simple FDEs considered here, one can develop spectral methods to solve them with the same kind of computational complexity and accuracy as one solves usual PDEs.

This is a first but important step towards developing efficient and accurate spectral methods for solving FDEs. While we have only considered a class of very simple prototypical FDEs, the general principles and the approximation results developed in this paper open up new possibilities for dealing with more general FDEs.

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