

# OPTIMAL ERROR ESTIMATES OF SPECTRAL PETROV–GALERKIN AND COLLOCATION METHODS FOR INITIAL VALUE PROBLEMS OF FRACTIONAL DIFFERENTIAL EQUATIONS\*

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**Abstract.** We present optimal error estimates for spectral Petrov–Galerkin methods and spectral collocation methods for linear fractional ordinary differential equations with initial value on a finite interval. We also develop Laguerre spectral Petrov–Galerkin methods and collocation methods for fractional equations on the half line. Numerical results confirm the error estimates.

**Key words.** end-point singularity, spectral Petrov–Galerkin, collocation, error estimate, Jacobi polynomials, Laguerre polynomials

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**1. Introduction.** Numerical methods for fractional differential equations have been investigated for decades; see, e.g., [8, 12, 33]. However, spectral methods for these equations have a rather short history since the solutions usually have some singular lower-order derivatives. The recent investigation of spectral methods for these singular problems is motivated by the following facts. First, all numerical methods for these problems are nonlocal as spectral methods are. For example, in finite difference methods, see, e.g., [33], and in finite element methods, see, e.g., [13, 18], data at almost all grids or all elements are exploited to approximate the integral operators at one grid or element. These methods are still nonlocal, even when a “fixed memory principle” is applied to reduce the use of all data; see, e.g., [15, 19]. Second, spectral methods lead to high-order accuracy when the solutions are smooth; see, e.g., [7, 24] for integer-order differential equations. For fractional differential equations with weakly singular kernels, solutions can be smooth even when some inputs of the equations are singular.

Consider the following fractional ordinary differential equation (FODE) over the interval  $I = (-1, 1)$ :

$$(1.1) \quad -_1\mathcal{D}_x^\mu(u - u_0) = f, \quad u(-1) = u_0, \quad 0 < \mu < 1,$$

where  $f \in L^p(I)$  ( $p \geq 1$ ) and  ${}_1\mathcal{D}_x^\mu$  is the left Riemann–Liouville fractional derivative defined by, see, e.g., [34],

$$(1.2) \quad -_1\mathcal{D}_x^\mu u(x) = \frac{d}{dx} {}_1\mathcal{I}_x^{1-\mu} u, \quad -_1\mathcal{I}_x^{1-\mu} u = \frac{1}{\Gamma(1-\mu)} \int_{-1}^x \frac{u(y)}{(x-y)^\mu} dy, \quad x > -1.$$

When the solutions to (1.1) are smooth, spectral methods lead to higher-order accuracy; see, e.g., [28, 45] for spectral Galerkin methods and, e.g., [16, 17, 26, 38] for

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spectral collocation methods. When the solutions to (1.1) are not smooth, spectral methods can also lead to high-order accuracy as the singularity is usually of the type  $(1+x)^\mu$ ; see, e.g., [8, Chapter 6]. To separate the singularity, we can approximate the solutions with the weighted basis  $(1+x)^\mu \mathbb{P}_N(I)$ , where  $\mathbb{P}_N(I)$  is the set of algebraic polynomials of order up to  $N$ . This fact has been used in [11] to present some Jacobi-spectral collocation methods for a linear Volterra integral equation of the second kind, to which (1.1) is equivalent under some conditions. See also [10, 41, 42, 43] for spectral Petrov–Galerkin methods and [44] for spectral collocation methods solving (1.1) with this weighted basis. However, there are no error estimates for spectral collocation methods in [44]. Here, we would provide such error estimates and use a different, unified, theoretical framework to present our error estimates than those for spectral and collocation methods in [10, 11]. The advantage of our error estimates is that we can fully take the endpoint singularity into account.

For (1.1), spectral methods are performed in the framework of Petrov–Galerkin methods to adapt to the nonsymmetric property of the integral operator; see [28] for smooth solutions and [42, 43] for singular solutions. Similar to the spectral Petrov–Galerkin methods for integer-order differential equations, see, e.g., [29, 35, 37], the error estimate of spectral Petrov–Galerkin methods for FODEs usually lies in some Jacobi-weighted spaces with negative weights; see, e.g., [42]. Usually, these weights can provide proper norms to incorporate singularities at endpoints.

In this work, we will present a *unified* numerical framework for (1.1) that can deal with both smooth and singular solutions, which is the *first point* of the paper. The singular solution can be with arbitrary singularity index at the end-point, i.e.,  $(1+x)^\beta$ , where  $\beta \geq 0$  and is not necessarily equal to  $\mu$ , the order of fractional derivatives. In this case, we require that the forcing term  $f$  either is smooth enough or only has singularity at endpoints. Here, we notice that there is another direction of unification of the Petrov–Galerkin methods—they have been extended from FODEs with one fractional derivative to multiterm fractional ordinary and partial differential equations with constant coefficients and smooth solutions in [41].

One of the key elements for Galerkin or Petrov–Galerkin methods is the fractional integration by parts for functions in Sobolev spaces. Here, we do not require vanishing boundary values, which extends similar formulas derived in [18, 28]. The argument is based on the characterization of the fractional Sobolev spaces; see, e.g., [34, Chapter 2] and section 2 in this paper. With the new fractional integration by parts, we can readily obtain the error estimate in different norms for the spectral methods, see Theorem 2.8, while the error estimate in [10] allows only the  $L^2$ -norm of the fractional derivative of order  $\mu$ . Further, with a Hardy-type inequality, we can reach the optimal error estimates in different norms.

In the spectral collocation methods, we also use the basis  $(1+x)^\beta \mathbb{P}_N(I)$  in the computation of differentiation matrix, and correspondingly the convergence order is the same with the spectral Petrov–Galerkin methods if the solution has somewhat higher regularity in weighted Sobolev spaces; see Theorems 2.8 and 2.9.

The *second point* of the paper is to present Laguerre spectral Petrov–Galerkin and collocation methods for FODEs on the half line. In this case, we have the same singularity at the left endpoint and also have singularity at infinity (the decay rate at infinity). Thus, we can extend the idea of solving FODEs on finite intervals when we know the singularity at infinity. However, we note that Laguerre spectral Petrov–Galerkin methods are only accurate on a short interval in the pointwise sense, while the weighted  $L^2$ -norms of the numerical errors are very small. This is because of the fast decaying weight  $\exp(-x)$  associated with the Laguerre polynomials. In this sense, we

need better knowledge on the decaying rate and corresponding spectral basis induced by slow decaying weights on the half line, e.g., mapped Jacobi polynomials and generalized Laguerre functions; see, e.g., [36]. However, we do not include such a discussion here due to the limit on the length of the paper. In the literature, spectral methods for FODEs on the half line have been investigated using the generalized Laguerre polynomials; see, e.g., [6] for Laguerre spectral methods and, e.g., [25] for Laguerre spectral collocation methods, without taking into account the endpoint singularity.

The main message of the paper is to show how to recover spectral accuracy from the endpoint singularity for simple FODEs like (1.1) using spectral methods with the approximation basis  $(1+x)^\mu \mathbb{P}_N(I)$ , following the ideas in [10, 11, 42, 43, 44]. In the literature, the endpoint singularity is resolved using a refined (nonuniform) grid at the endpoints, see, e.g., [9, 14, 30, 31], which can lead to uniform algebraic convergence of numerical methods for general FODEs including (1.1). Here, we investigate the possibility of obtaining faster convergence in certain cases. For general FODEs of complicated forms, such as FODEs with multiterm fractional derivatives and fractional partial differential equations with time or space fractional derivatives, the approximation basis  $(1+x)^{\mu/2} \mathbb{P}_N(I)$  has been proposed for smooth solutions in [41]. We believe that our study is a starting point for the development of truly high-order methods for general FODEs whose solutions can be either smooth or singular.

The rest of the paper is organized as follows. In section 2, we focus on the scalar FODE (1.1) over the interval  $I = (-1, 1)$ . We prove the formula of integration by parts, the well-posedness in fractional Sobolev spaces, and the regularity in weighted Sobolev spaces. We present error estimates for spectral Petrov–Galerkin/Galerkin methods and spectral collocation methods, the proofs of which can be found in section 5. In section 3, we consider spectral Petrov–Galerkin/Galerkin methods and collocation methods for FODEs on the half line  $\Lambda = (0, \infty)$ . In section 4, we show some numerical results that confirm our error estimates. We conclude and discuss our approach in section 6.

**2. Spectral Petrov–Galerkin and collocation methods on finite intervals.** Consider the FODE (1.1) over the interval  $I = (-1, 1)$ . Assume that  $f \in L^p(I)$  for some  $p \geq 1$ . By (A.1) and (A.4) in Appendix A, (1.1) can be equivalently formulated as

$$(2.1) \quad u(x) = u_0 + c(x+1)^{\mu-1} + {}_{-1}\mathcal{I}_x^\mu f,$$

where  $c$  is an arbitrary constant. To ensure continuity at  $x = -1$ , i.e.,  $\lim_{x \rightarrow -1} u(x) = u_0$ , we require the following consistency condition:

$$(2.2) \quad c = 0, \text{ and } \lim_{x \rightarrow -1} {}_{-1}\mathcal{I}_x^\mu f = 0.$$

For simplicity, we consider  $u(-1) = u_0 = 0$ . Then

$$(2.3) \quad u(x) = {}_{-1}\mathcal{I}_x^\mu f.$$

*Remark 2.1.* Here, we use the modified Riemann–Liouville fractional derivative in (1.1), which is equivalent to the Caputo fractional derivative  ${}^C_{-1}\mathcal{D}_x^\mu u = {}_{-1}\mathcal{I}_x^\mu \partial_x u$  when  $u$  is continuous over  $[-1, 1]$  and  $f \in L^\infty([-1, 1])$ . If the Caputo derivative is used in (1.1) in place of the modified Riemann–Liouville fractional derivative, we then have  ${}_{-1}\mathcal{I}_x^\mu [\partial_x u] = f$ ,  $f \in L^\infty([-1, 1])$ . We then have the same solution as in (2.1) when  $u$  is continuous ( $c = 0$ ). In fact, by Lemma 2.22 in [34], taking  ${}_{-1}\mathcal{I}_x^\mu$  over both

sides of this equation gives  $u = u_0 + {}_{-1}\mathcal{I}_x^\mu f$ , which is (2.1) with  $c = 0$ . From Lemma 2.21 in [34], we know that

$${}_{-1}\mathcal{D}_x^\mu[u_0 + {}_{-1}\mathcal{I}_x^\mu f] = {}_{-1}\mathcal{D}_x^\mu {}_{-1}\mathcal{I}_x^\mu f = f$$

when  $f \in L^\infty([-1, 1])$ .

**2.1. Regularity.** Denote by  $H^\mu(I)$  the standard Sobolev–Hilbert space of fractional order  $\mu$  and  ${}_0H^\mu(I) = \{v|v \in H^\mu(I), v(-1) = 0, \mu > 1/2\}$ . For the solution to (1.1), we have the following regularity. The proof can be found in section 5.

**THEOREM 2.2** (regularity). *For  $f \in L^p(I)$ ,  $p > 1/\mu$  and  $0 < \mu < 1$ , and then  $u \in {}_0H^{\mu+1/2-1/p}(I)$ .*

In the literature, the regularity has also been considered the space  $J_L^\mu(I)$ , see, e.g., [10, 18, 28], defined by

$$(2.4) \quad \{v|v, {}_{-1}\mathcal{D}_x^\mu v \in L^2(I)\}$$

and equipped with the norm  $\|u\|_{J_L^\mu} = (\|{}_{-1}\mathcal{D}_x^\mu u\|^2 + \|u\|^2)^{1/2}$ . This space can be shown to be very close to the classical Sobolev–Hilbert space  $H^\mu(I)$  as follows.

**PROPOSITION 2.3.** *If  $0 < \mu < 1/2$ , we have  $J_L^\mu(I) = H^\mu(I)$ . For  $1/2 < \mu < 1$ , we have*

$$(2.5) \quad J_L^\mu(I) = {}_0H^\mu(I) \oplus \{(x + 1)^{\mu-1}\}.$$

We only consider the classical Sobolev–Hilbert spaces hereafter.

It is true that  $u$  does not have high regularity in standard Sobolev spaces, but it may have high regularity in the weighted Sobolev spaces. For example, when  $f = 1 \in H^\infty(I)$ ,  $u = \frac{(1+x)^\mu}{\Gamma(1+\mu)}$  does not belong to  $H^1(I)$  if  $0 < \mu \leq 1/2$ , while if  $1/2 < \mu < 1$ ,  $u$  does belong to  $H^1(I)$  but does not belong to  $H^2(I)$ . However, we note that  $(1+x)^{-\mu}u$  are in  $H^\infty(I)$ . This suggests the separation of singularity (of derivatives of  $u$ ) at the left endpoint in order to have higher regularity where spectral methods can be effective.

To better incorporate singularities at the endpoints, we introduce the following weighted Sobolev space, see, e.g., [10, 21],

$$(2.6) \quad B_{\omega^{\alpha,\beta}}^m(I) := \{u|\partial_x^k u \in L_{\omega^{\alpha+k,\beta+k}}^2(I), k = 0, 1, \dots, m\},$$

$m$  is a nonnegative integer

with  $\omega^{\alpha,\beta} = (1-x)^\alpha(1+x)^\beta$ ,  $\alpha, \beta > -1$ , which is equipped with the following norm:

$$(2.7) \quad \|u\|_{m,\omega^{\alpha,\beta},B} = \left( \sum_{k=0}^m |u|_{k,\omega^{\alpha,\beta},B}^2 \right)^{1/2}, \quad |u|_{k,\omega^{\alpha,\beta},B} = \|\partial_x^k u\|_{\omega^{\alpha+k,\beta+k}}.$$

When  $m$  is not an integer, the space is defined by interpolation; see, e.g., [21].

We have the following regularity in weighted Sobolev spaces.

**THEOREM 2.4** (regularity in weighted Sobolev spaces). *Assume that  $u(-1) = 0$  and  $\alpha > \mu - 1$ . If  $\omega^{0,\mu-\beta} f \in B_{\omega^{\alpha,\beta-\mu}}^r(I)$  ( $r \geq 0$ ) with  $\beta > 1 - \mu$  or  $\omega^{0,\mu-\beta} f \in B_{\omega^{\alpha,\beta-\mu}}^r(I) \cap C(\bar{I})$  ( $r \geq 1$ ), then  $\omega^{0,-\beta}u \in B_{\omega^{\alpha-\mu,\beta}}^{r+\mu}(I)$ . Here  $C(\bar{I})$  denotes the space of continuous functions with the maximum norm on the closed interval  $\bar{I}$ .*

The right Riemann–Liouville derivative  ${}_x\mathcal{D}_1^\mu v$  is defined by, see, e.g., [34],

$${}_x\mathcal{D}_1^\mu v = -\frac{1}{\Gamma(1-\mu)} \frac{d}{dx} \int_x^1 \frac{v(y)}{(y-x)^\mu} dy.$$

We have the following integration by parts for functions in standard Sobolev spaces.

THEOREM 2.5 (integration by parts in Sobolev spaces). *Supposing that  $u \in H^\mu(I)$ ,  $0 < \mu < 1$ , and  $v \in H^{\mu_2}(I)$ , it holds that*

$$(2.8) \quad (-_1\mathcal{D}_x^\mu u, v) = (-_1\mathcal{D}_x^{\mu_1} u, {}_x\mathcal{D}_1^{\mu_2} v),$$

where  $0 \leq \mu_1, \mu_2 \leq \mu$ , and  $\mu_1 + \mu_2 = \mu$ .

Now we can present our scheme for (1.1). Denote the collection of algebraic polynomials of order up to  $N$  by  $\mathbb{P}_N(I)$ . Define the following finite-dimensional spaces for  $\alpha, \beta > -1$ :

$$(2.9) \quad X_N^\beta = \{u | u = (1+x)^\beta v, v \in \mathbb{P}_N(I)\}, \quad Y_N^\alpha = \{u | u = (1-x)^\alpha v, v \in \mathbb{P}_N(I)\}.$$

Here, we call  $\beta$  the singularity index of the trial basis  $X_N^\beta$ , which will be chosen according to the singularity of the forcing term in (1.1). Our spectral Petrov–Galerkin method is to find  $u_N \in X_N^\beta$  such that for all  $v \in Y_N^\alpha$ ,

$$(2.10) \quad (-_1\mathcal{D}_x^{\mu_1} u_N, {}_x\mathcal{D}_1^{\mu_2} v) = (f, v),$$

where  $0 \leq \mu_1, \mu_2 \leq \mu$ ,  $\mu_1 + \mu_2 = \mu$ , and  $\alpha, \beta > \mu - 1$  will be chosen according to the forcing term  $f$ . If there exists a constant  $\sigma$  such that  $(1+x)^{-\sigma} f$  has better regularity in the aforementioned weighted Sobolev spaces than  $f$  does, then we choose  $\beta$  as the fractional part of  $\sigma + \mu$ . The constant  $\alpha$  should be chosen such that  $\alpha > 1 - \mu$ . In section 4, we show numerically that the choice of  $\beta = \sigma + \mu - [\sigma + \mu]$  ( $[\sigma + \mu]$  is the integer part of  $\sigma + \mu$ ) leads to better accuracy than taking  $\beta = \mu$  in [10, 43].

In practice, we may use a weighted  $L^2$ -projection or numerical integration on the right-hand side of the scheme (2.10). Specifically, we use either of the following formulations:

$$(2.11) \quad (-_1\mathcal{D}_x^{\mu_1} u_N, {}_x\mathcal{D}_1^{\mu_2} v) = (\omega^{0, \beta - \mu} \pi_N^{\alpha, \beta - \mu} [\omega^{0, \mu - \beta} f], v),$$

where  $\pi_N^{\alpha, \beta}$  is the  $L^2_{w^{\alpha, \beta}}(I)$ -orthogonal projection

$$(2.12) \quad (\pi_N^{\alpha, \beta} u - u, v)_{w^{\alpha, \beta}} = 0 \quad \forall v \in \mathbb{P}_N(I),$$

and

$$(2.13) \quad (-_1\mathcal{D}_x^{\mu_1} u_N, {}_x\mathcal{D}_1^{\mu_2} v) = (\omega^{0, \beta - \mu} \mathcal{I}_N^{\alpha, \beta - \mu} [\omega^{0, \mu - \beta} f], v),$$

where  $\mathcal{I}_N^{\alpha, \beta - \mu}$  is the Gauss–Jacobi interpolation operator which is induced by the Lagrange polynomial interpolation using the  $N + 1$  roots of the Jacobi polynomial  $P_{N+1}^{\alpha, \beta - \mu}(I)$ .

To efficiently implement the scheme (2.10), we are looking for  $u_N, v$  of the form

$$(2.14) \quad u_N = (1+x)^\beta \sum_{n=0}^N u_n P_n^{\alpha - \mu, \beta}, \quad v = (1-x)^\alpha P_j^{\alpha, \beta - \mu}, \quad j = 0, 1, \dots, N,$$

where  $\alpha, \beta > \mu - 1$ . Then, by (B.5) and (B.6) of Appendix A,

$$u_j = \frac{(2j + \alpha + \beta - \mu + 1)j!\Gamma(j + \alpha + \beta - \mu + 1)}{2^{\alpha + \beta - \mu + 1}\Gamma(\alpha + j + 1)\Gamma(\beta + j + 1)}(f, v_j), \quad j = 0, 1, \dots, N.$$

*Remark 2.6.* When  $\alpha = \beta = 0$ , we have a Galerkin method instead of a Petrov–Galerkin method as  $X_N^0 = Y_N^0$ . When  $\alpha = \beta = \mu/2$  in (2.10), we recover the Petrov–Galerkin method proposed in [43]. When  $\alpha = \beta = 1$  in (2.10), we recover the Petrov–Galerkin method in time proposed in [28].

According to Theorem 2.5,  $\mu_1, \mu_2$  can be any values that satisfy the requirements, i.e.,  $\mu_1, \mu_2 \geq 0$  and  $\mu_1 + \mu_2 = \mu$ . However, once we employ the expansions in (2.14) in the scheme (2.10), the resulting linear systems are the same regardless of the values of  $\mu_1$  and  $\mu_2$ . We note that the formula (2.8) is useful in deriving our error estimates.

Now, we consider spectral collocation methods. Define  $\mathcal{I}_{N,\beta}^{\delta,\gamma} u = \omega^{0,\beta} \mathcal{I}_N^{\delta,\gamma} [\omega^{0,-\beta} u]$ , where  $\mathcal{I}_N^{\delta,\gamma}$  ( $\delta, \gamma > -1$ ) is the Gauss–Jacobi interpolation operator induced by the  $N + 1$  roots of the Jacobi polynomial  $P_{N+1}^{\delta,\gamma}(I)$ . By the definition of  $\mathcal{I}_{N,\beta}^{\delta,\gamma}$ , we have

$$(2.15) \quad \mathcal{I}_N^{\delta,\gamma} u \in \mathbb{P}_N(I), \quad \mathcal{I}_{N,\beta}^{\delta,\gamma} u = \omega^{0,\beta} \mathcal{I}_N^{\delta,\gamma} [\omega^{0,-\beta} u] \in X_N^\beta.$$

Our *spectral collocation method* for (1.1) is to find  $u_N \in X_N^\beta$  such that

$$(2.16) \quad -_1\mathcal{D}_x^\mu(\mathcal{I}_{N,\beta}^{\delta,\gamma} u_N) - \mathcal{I}_{N,\beta-\mu}^{\delta,\gamma} f = 0, \quad \delta, \gamma > -1, \beta \geq 0.$$

This method extends the collocation method proposed in [44], where  $\beta = 1 + \mu$  and it is required that  $\lim_{x \rightarrow -1} (1 + x)^{-1-\mu} u_N$  exists. Here, we only require that in (2.16),  $\lim_{x \rightarrow -1} (1 + x)^{-\beta} u_N$  exists, where  $\beta$  is taken less than one.

In implementation, we use the following representation:

$$(2.17) \quad u_N = \sum_{j=1}^{N+1} u_N(x_j) \left( \frac{x+1}{x_j+1} \right)^\beta l_j(x), \quad l_j(x) = \prod_{k=1, \dots, N+1, k \neq j} \frac{x-x_k}{x_j-x_k}.$$

As in standard spectral collocation methods, see, e.g., [24], we write

$$(2.18) \quad l_j(x) = \sum_{k=0}^N B_{k,j} P_k^{\delta,\beta}(x).$$

Then, by (2.17), (2.18), and (B.5), we have

$$-_1\mathcal{D}_x^\mu u_N = (1+x)^{\beta-\mu} \sum_{j=1}^{N+1} \frac{u_N(x_j)}{(x_j+1)^\beta} \sum_{k=0}^N B_{k,j} \frac{\Gamma(n+1+\beta)}{\Gamma(n+1+\beta-\mu)} P_k^{\delta+\mu,\beta-\mu}(x).$$

We introduce the differentiation matrix  $D$  such that

$$(2.19) \quad D\vec{u} = \vec{f},$$

where we use the Gauss–Jacobi quadrature points (roots of the Jacobi polynomial  $P_{N+1}^{\delta,\gamma}(x)$ ) and

$$\begin{aligned} \vec{u} &= ((x_1+1)^{-\beta} u_N(x_1), \dots, (x_{N+1}+1)^{-\beta} u_N(x_{N+1}))^\top, \\ \vec{f} &= ((x_1+1)^{\mu-\beta} f(x_1), \dots, (x_{N+1}+1)^{\mu-\beta} f(x_{N+1}))^\top, \\ D_{i,j} &= \sum_{k=0}^{N-1} B_{k,j} \frac{\Gamma(n+1+\beta)}{\Gamma(n+1+\beta-\mu)} P_k^{\delta+\mu,\beta-\mu}(x_i). \end{aligned}$$

*Remark 2.7.* Here we use the Gauss–Jacobi quadrature points. The equispaced points should be avoided since the linear system for  $B_{k,j}$  in (2.18) is then ill-posed; see, e.g., [44] for numerical illustrations of fast growth of condition numbers of the linear system.

We note that  $O(N \log(N))$  fast algorithms can be applied to obtain  $B_{k,j}$ ; see, e.g., [2] for  $\beta = \delta = 0$  and [27, 32] for  $\beta, \delta > -1$  when  $x_j$  are Gauss–Chebyshev quadrature points  $\delta = \gamma = -1/2$ .

We now present the *error estimates* for our spectral method (2.10) and spectral collocation method (2.16). The proofs can be found in section 5.

**THEOREM 2.8** (convergence rate of spectral Petrov–Galerkin methods). *Suppose that  $u$  is the solution to (1.1) and  $u_N \in X_N^\beta$  is the solution to (2.11). Under the assumptions in Theorem 2.4, it holds that for any  $0 \leq \mu_1 \leq \mu$ ,*

$$(2.20) \quad \left\| {}_{-1}\mathcal{D}_x^{\mu_1} u_N \right\|_{\omega^{\alpha-\mu+\mu_1, \mu_1-\beta}} \leq \left\| {}_{-1}\mathcal{I}_x^{\mu-\mu_1} [\omega^{0, \beta-\mu} \pi_N^{\alpha, \beta-\mu} [\omega^{0, \mu-\beta} f]] \right\|_{\omega^{\alpha-\mu+\mu_1, \mu_1-\beta}}$$

and

$$(2.21) \quad \left\| {}_{-1}\mathcal{D}_x^{\mu_1} (u - u_N) \right\|_{\omega^{\alpha-\mu+\mu_1, \mu_1-\beta}} \leq CN^{-r-\mu+\mu_1} \left\| \partial_x^r [\omega^{0, \mu-\beta} f] \right\|_{\omega^{\alpha+r, \beta-\mu+r}}.$$

When  $\mu_1 = 0$ ,  $\alpha \leq \mu$ , and  $\beta \geq 0$ , we have the  $L^2$ -estimate

$$\|u - u_N\| \leq \|u - u_N\|_{\omega^{\alpha-\mu, -\beta}} \leq CN^{-r-\mu} \left\| \partial_x^r [\omega^{0, \mu-\beta} f] \right\|_{\omega^{\alpha+r, \beta-\mu+r}}.$$

**THEOREM 2.9** (convergence rate of spectral collocation methods). *Suppose that  $\omega^{0, \mu-\beta} f \in B_{\alpha, \beta-\mu}^r(I) \cap C(\bar{I})$ ,  $r \geq 1$ , and  $u_0 = 0$ . Then, for  $-1 < \delta \leq \alpha \leq \delta + 1$  and  $-1 < \gamma \leq \beta - \mu \leq \gamma + 1$ , we have that for  $0 \leq \mu_1 \leq \mu$ , there exists a constant  $C > 0$  independent of  $N$  such that*

$$(2.22) \quad \left\| {}_{-1}\mathcal{D}_x^{\mu_1} (u_N - u) \right\|_{\omega^{\alpha-\mu+\mu_1, -\beta+\mu_1}} \leq CN^{-r-\mu+\mu_1} \left\| \partial_x^r [\omega^{0, \mu-\beta} f] \right\|_{\omega^{\alpha+r, \beta-\mu+r}},$$

where  $\delta, \gamma$  are from (2.16).

**3. Spectral Petrov–Galerkin and collocation methods on the half line.**

We now consider the following FODE over the half line  $\Lambda = \{x | 0 < x < \infty\}$ :

$$(3.1) \quad {}_0\mathcal{D}_x^\mu (u - u_0) = f, \quad u(0) = u_0, \quad 0 < \mu < 1.$$

When the domain is  $(a, \infty)$  ( $-\infty < a < \infty$ ), we can shift the domain to  $\Lambda$  by a linear transformation. Let  $f \in L^p(\Lambda)$  for any  $p \geq 1$ . By the fact (see, e.g., [34, section 6])

$${}_0\mathcal{D}_x^\mu {}_0\mathcal{I}_x^\mu v = v, \quad \forall v \in L^1(\Lambda)$$

and the fact that  ${}_0\mathcal{D}_x^\mu v = 0$  is equivalent to  $v = cx^{\mu-1}$  ( $c$  is a constant), we have

$$(3.2) \quad u = u_0 + cx^{\mu-1} + {}_0\mathcal{I}_x^\mu f.$$

For simplicity, we consider only the following case:  $u_0 = c = 0$  while the general case can be considered by introducing an auxiliary function  $\hat{u} = u - u_0 - cx^{\mu-1}$ .

To approximate the solution to (3.1), we use the generalized Laguerre polynomials introduced in [23]

$$(3.3) \quad L_n^{\alpha, \beta}(x) = \frac{x^{-\beta} e^{\alpha x}}{n!} \frac{d^n}{dx^n} (e^{-\alpha x} x^{n+\beta}), \quad \beta > -1, \alpha > 0.$$

These polynomials form a complete orthogonal basis in  $L^2_{\rho^{\alpha,\beta}}(\Lambda)$ , where  $\rho^{\alpha,\beta} := \rho^{\alpha,\beta}(x) = e^{-\alpha x}x^\beta$  and

$$(3.4) \quad \int_{\Lambda} L_n^{\alpha,\beta}(x)L_m^{\alpha,\beta}(x)\rho^{\alpha,\beta}(x) dx = \frac{\Gamma(n + \beta + 1)}{\alpha^{\beta+1}n!}\delta_{n,m}.$$

The space  $L^2_{\rho^{\alpha,\beta}}(\Lambda)$  is defined by

$$L^2_{\rho^{\alpha,\beta}}(\Lambda) = \left\{ v \mid v \text{ is measurable on } \Lambda \text{ and } \|v\|_{\rho^{\alpha,\beta}} < \infty \right\}$$

with the following inner product and norm:

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

The derivatives of the generalized Laguerre polynomials are still generalized Laguerre polynomials:

$$\partial_x L_n^{\alpha,\beta}(x) = -\alpha L_{n-1}^{\alpha,\beta+1}(x).$$

Denote  $L_n^\beta(x) = L_n^{1,\beta}(x)$ . It can be readily checked that  $L_n^{\alpha,\beta}(x) = L_n^\beta(\alpha x)$ .

Define also the right Riemann–Liouville derivative  ${}_x\mathcal{D}_\infty^\mu v$ , see, e.g., [34],

$${}_x\mathcal{D}_\infty^\mu v = -\frac{1}{\Gamma(1 - \mu)} \frac{d}{dx} \int_x^\infty \frac{v(y)}{(y - x)^\mu} dy.$$

LEMMA 3.1. *For  $\mu > 0$  and  $\alpha > 0$ , we have, for any  $x > 0$ ,*

$$(3.5) \quad {}_0\mathcal{I}_x^\mu(x^\beta L_n^{\alpha,\beta}(x)) = \frac{\Gamma(n + \beta + \mu + 1)}{\Gamma(n + \beta + 1)} x^{\beta+\mu} L_n^{\alpha,\beta+\mu}(x), \beta > -1,$$

$$(3.6) \quad {}_x\mathcal{I}_\infty^\mu(e^{-\alpha x} L_n^{\alpha,\beta+\mu}(x)) = \alpha^{-\mu} e^{-\alpha x} L_n^{\alpha,\beta}(x), \beta > -1,$$

$$(3.7) \quad {}_0\mathcal{D}_x^\mu(x^\beta L_n^{\alpha,\beta}(x)) = \frac{\Gamma(n + \beta - \mu + 1)}{\Gamma(n + \beta + 1)} x^{\beta-\mu} L_n^{\alpha,\beta-\mu}(x), \beta > \mu - 1,$$

$$(3.8) \quad {}_x\mathcal{D}_\infty^\mu(e^{-\alpha x} L_n^{\alpha,\beta}(x)) = \alpha^\mu e^{-\alpha x} L_n^{\alpha,\beta+\mu}(x), \beta > -1.$$

See, e.g., [3, 5] for the proof of the identity (3.5). The identity (3.6) can be proved using the completeness of the generalized Laguerre polynomials; see, e.g., [5]. The relations (3.7) and (3.8) follow immediately from (A.2) (with a slight modification on the endpoint of the interval), (3.5), and (3.6).

We need the following integration-by-parts formula for our spectral methods.

LEMMA 3.2 (integration by parts on a the half line). *Suppose that  $f = {}_0\mathcal{I}_x^\mu \phi$ ,  $\phi \in L^p(\Lambda)$ , and that  $g = {}_x\mathcal{I}_\infty^{\mu_2} \psi$ ,  $\psi \in L^q(\Lambda)$ , where  $1/p + 1/q = 1 + \mu$  and  $p, q > 1$ . Then, for any  $0 < \mu < 1$ , it holds that*

$$(3.9) \quad ({}_0\mathcal{D}_x^\mu f, g) = ({}_0\mathcal{D}_x^{\mu_1} f, {}_x\mathcal{D}_\infty^{\mu_2} g),$$

where  $0 \leq \mu_1, \mu_2 \leq \mu$ , and  $\mu_1 + \mu_2 = \mu$ .

Denote by  $\mathbb{P}_N(\Lambda)$  the set of algebraic polynomials of order up to  $N$  over  $\Lambda$  and

$$(3.10) \quad Z_N^\beta = \{w \mid w = x^\beta v, v \in \mathbb{P}_N(\Lambda), \beta \geq 0\}.$$

When  $\beta \geq 0$ , the space  $\rho^{\alpha,0}\mathbb{P}_N(\Lambda)$  is a subspace of  $L^p(\Lambda)$  for any  $p \geq 1$  and there exists  $\psi \in L^q(\Lambda)$  ( $q \geq 1$ ) for any  $g \in \rho^{\alpha,0}\mathbb{P}_N(\Lambda)$  such that  $g = {}_x\mathcal{I}_\infty^{\mu_2} \psi$ . Then, by



Lemma 3.2, our spectral Petrov–Galerkin method is to find  $u_N \in Z_N^\beta$  such that for any  $v_N \in \mathbb{P}_N(\Lambda)$ , we have

$$(3.11) \quad ({}_0\mathcal{D}_x^{\mu_1} u_N, {}_x\mathcal{D}_\infty^{\mu_2} (v_N \rho^{\alpha,0})) = (f, v_N) = (x^{\alpha-\mu} \Pi_N^{\alpha,\beta-\mu} x^{\mu-\beta} f, v_N)_{\rho^{\alpha,0}}.$$

In (3.11), we write  $u_N = x^\beta \sum_{n=0}^N u_n L_n^{\alpha,\beta}(x)$  and take  $v_N$  from the set  $\{L_j^{\alpha,\beta-\mu}\}_{j=0}^N$ . We then obtain

$$\sum_{n=0}^N u_n ({}_0\mathcal{D}_x^{\mu_1} [x^\beta L_n^{\alpha,\beta}(x)], {}_x\mathcal{D}_\infty^{\mu_2} (L_j^{\alpha,\beta-\mu} \rho^{\alpha,0})) = (f, L_j^{\alpha,\beta-\mu})_{\rho^{\alpha,0}}, \quad j = 0, 1, \dots, N.$$

Then, by Lemma 3.1 and orthogonality of the generalized Laguerre polynomials (3.4), we have

$$(3.12) \quad u_j = \frac{\alpha^{\beta-\mu+1} \Gamma(j+1)}{\Gamma(j+\beta+1)} (f, L_j^{\alpha,\beta-\mu})_{\rho^{\alpha,0}}, \quad j = 0, 1, \dots, N.$$

Now, we consider spectral collocation methods. Define  $\mathfrak{J}_{N,\beta}^{\delta,\gamma} u = x^\beta \mathfrak{J}_N^{\delta,\gamma} [x^{-\beta} u]$ , where  $\mathfrak{J}_N^{\delta,\gamma}$  is the Gauss–Laguerre interpolation operator associated with the  $N + 1$  roots of  $L_{N+1}^{\delta,\gamma}(x)$ . By the definition of  $\mathfrak{J}_{N,\beta}^{\delta,\gamma}$ , we have

$$(3.13) \quad \mathfrak{J}_N^{\delta,\gamma} u \in \mathbb{P}_N(\Lambda), \quad \mathfrak{J}_{N,\beta}^{\delta,\gamma} u \in Z_N^\beta.$$

Our spectral collocation method for (3.1) is to find  $u_N \in Z_N^\beta$  such that

$$(3.14) \quad -{}_1\mathcal{D}_x^\mu (\mathfrak{J}_{N,\beta}^{\delta,\gamma} u_N) - \mathfrak{J}_{N,\beta-\mu}^{\delta,\gamma} f = 0, \quad -1 < \beta \leq 1.$$

In implementation, we use the following representation:

$$u_N = \sum_{j=1}^{N+1} u_N(x_j) \left(\frac{x}{x_j}\right)^\beta l_j(x), \quad l_j(x) = \prod_{k=1, \dots, N+1, k \neq j} \frac{x - x_k}{x_j - x_k}.$$

We write  $l_j(x) = \sum_{k=0}^{N-1} B_{k,j} L_k^{\alpha,\beta}(x)$ , where  $B_{k,j}$  can be uniquely determined by  $B_{k,j} = \alpha^{\beta+1} n! (L_k^{\alpha,\beta}, l_j)_{\rho^{\alpha,\beta}} / \Gamma(n + \beta + 1)$ . Then, by (B.5), we have

$$(3.15) \quad {}_0\mathcal{D}_x^\mu u_N = x^{\beta-\mu} \sum_{j=1}^{N+1} u_N(x_j) x_j^{-\beta} \sum_{k=0}^N B_{k,j} \frac{\Gamma(n+1+\beta)}{\Gamma(n+1+\beta-\mu)} L_k^{\alpha,\beta-\mu}(x).$$

We introduce the differentiation matrix  $D$  such that

$$(3.16) \quad D \vec{u} = \vec{f},$$

where  $\vec{u} = (x_1^{-\beta} u_N(x_1), \dots, x_N^{-\beta} u_N(x_N))^\top$ ,  $\vec{f} = (x_1^{\mu-\beta} f(x_1), \dots, x_{N+1}^{\mu-\beta} f(x_{N+1}))^\top$ , and

$$D_{i,j} = \sum_{k=0}^{N-1} B_{k,j} \frac{\Gamma(n+1+\beta)}{\Gamma(n+1+\beta-\mu)} L_k^{\alpha,\beta-\mu}(x_i),$$

where  $x_i$  are the  $N + 1$  roots of the generalized polynomials  $L_{N+1}^{\delta,\gamma}(x)$ .

To present our error estimate, we need the following weighted space, see, e.g., [22],

$$A_{\alpha,\beta}^r(\Lambda) = \left\{ v | \partial_x^k v \in L_{\rho^{\alpha,\beta+k}}^2(\Lambda), k = 0, 1, 2, \dots, r \right\},$$

which is equipped with the norm  $\|v\|_{A_{\alpha,\beta}^r} = (\sum_{k=0}^r \|\partial_k v\|_{\rho^{\alpha,\beta+k}}^2)^{1/2}$ .

**THEOREM 3.3** (convergence rate of spectral Petrov–Galerkin methods on the half line). *Suppose that  $u_0 = 0$  and  $\rho^{0,\mu-\beta} f$  in  $A_{\alpha,\mu-\beta}^r(\Lambda)$ . Then, for  $0 \leq \mu_1 \leq \mu$ ,*

$$(3.17) \quad \|{}_0\mathcal{D}_x^{\mu_1}(u - u_N)\|_{\rho^{\alpha,\mu_1-\beta}} \leq C(\alpha N)^{(-r-\mu+\mu_1)/2} \|\partial_x^r(\rho^{0,\mu-\beta} f)\|_{\rho^{\alpha,\beta-\mu+r}}.$$

**THEOREM 3.4** (convergence rate of spectral collocation methods on the half line). *For  $\rho^{0,\mu-\beta} f \in A_{\alpha,\beta}^r(\Lambda) \cap A_{\alpha-1,\beta}^r(\Lambda)$  and any integer  $r \geq 1$ , we have when  $u_0 = 0$  that*

$$(3.18) \quad \|u_N - u\|_{\rho^{\alpha,-\beta}} \leq C(\alpha N)^{(1-r-\mu)/2} \left( \alpha^{-1} \|\partial_x^r[\rho^{0,\mu-\beta} f]\|_{\rho^{\alpha,\beta+r-1}} + (1 + \alpha^{-1/2})(\ln N)^{1/2} \|\partial_x^r[\rho^{0,\mu-\beta} f]\|_{\rho^{\alpha,\beta+r}} \right).$$

**4. Numerical results.** In this section, we will test the spectral Petrov–Galerkin methods and the spectral collocation methods for linear single-term fractional differential equations on both the finite interval and the half line. Our numerical results show the expected spectral convergence when the singularity index  $\beta$  is chosen properly.

**4.1. Finite interval.** Here, we test the spectral Petrov–Galerkin method using numerical integration on the right-hand side (2.13) and the spectral collocation method using (2.19). In (1.1), we take  $u_0 = 0$  and the right-hand side as follows:

$$\text{Case I : } f = (1 + x)^\sigma \sin(x); \quad \text{Case II : } f = (1 + x)^\sigma |x|^5; \quad \text{Case III: } f = \sin(1 + x).$$

The errors are measured in the following sense:

$$(4.1) \quad \varrho_\infty^r = \frac{\|u_N - u_{\text{ref}}\|_\infty}{\|u_{\text{ref}}\|_\infty},$$

where  $\|v\|_\infty = \max_{1 \leq j \leq M+1} |v(y_j)|$ ,  $y_j = -1 + 2(j-1)/M$ ,  $M = 20000$ . The reference  $u_{\text{ref}}$  is obtained by the same solver but with finer resolution. For spectral Petrov–Galerkin methods, we take  $N = 128$  in (2.13) to obtain the reference solution. For spectral collocation methods, we take  $N = 128$  in (2.19) to obtain the reference solution at the Gauss–Jacobi quadrature points and then obtain the value of  $u_{\text{ref}}$  at  $y_j$  through the Lagrange polynomial interpolation.

*Example 4.1* (Petrov–Galerkin method). In the Petrov–Galerkin method (2.10), we use numerical integration on the right-hand side, i.e., the formula (2.13). In the spectral Petrov–Galerkin method (2.13), we can use any  $\mu_1, \mu_2$  when  $\mu_1, \mu_2 \geq 0$  and  $\mu_1 + \mu_2 = \mu$  without changing the results; see Remark 2.6.

In all the cases, we test  $\alpha = -\mu, 0, \mu$  in the test basis  $Y_N^\alpha$  in (2.9) whenever  $\alpha > \mu - 1$ . The numerical results show that the errors are of the same magnitude, so we will only present the errors for  $\alpha = 0$ .

In Table 1, we observe that the relative errors go quickly to the machine precision when we have the proper singularity index of the solution, i.e., we take  $\beta = \sigma + \mu - [\sigma + \mu]$ . ( $[\sigma + \mu]$  is the integer part of  $\sigma + \mu$ .) Note that  $(1 + x)^{-\sigma} f$  is analytic, and by Theorem 2.4 we have that  $(1 + x)^{-\sigma-\mu} u$  is infinitely differentiable. Then, by

TABLE 1

Spectral Petrov–Galerkin methods, Case I with  $\mu = 0.2, \sigma = 0.2$ , relative  $L^\infty$  error:  $\beta = \sigma + \mu - \lfloor \sigma + \mu \rfloor$  (left) and  $\beta = \mu$  (right).

# Nodes	$\varrho_\infty^r$	$\varrho_\infty^r$	Order
4	5.9970e-04	8.2398e-02	
16	3.1781e-15	3.1565e-02	0.69
32	4.6348e-15	1.6522e-02	0.93
64	4.6348e-15	6.4508e-03	1.36

TABLE 2

Spectral Petrov–Galerkin methods, Case II with  $\mu = 0.8, \sigma = 0.5$ , relative  $L^\infty$  error:  $\beta = \sigma + \mu - \lfloor \sigma + \mu \rfloor$  (left) and  $\beta = \mu$  (right).

# Nodes	$\varrho_\infty^r$	Order	$\varrho_\infty^r$	Order
4	6.6170e-02		3.6445e-02	
16	5.1218e-06	6.83	7.5350e-04	2.80
32	9.0505e-08	5.82	1.3236e-04	2.51
64	1.6887e-09	5.74	2.1956e-05	2.59

TABLE 3

Spectral Petrov–Galerkin methods, Case III, relative  $L^\infty$  error:  $\beta = \mu = 0.2$  (left) and  $\beta = \mu = 0.8$  (right).

# Nodes	$\varrho_\infty^r$	$\varrho_\infty^r$
4	2.3844e-04	3.7597e-05
16	4.4016e-15	4.2813e-15

Theorem 2.8, we have exponential convergence as observed here. When taking  $\beta = \mu$ , we cannot reach the singularity index of the solution:  $(1+x)^{-\mu}u \in B_{\omega^{\mu,-\mu}}^{2\sigma+\mu+1-\epsilon}(I)$ , by  $f \in H^{2\sigma+1-\epsilon}(I)$  and Theorem 2.4. Thus, we can only expect algebraic convergence with rate  $2\sigma + \mu + 1 - \epsilon$  ( $1.6 - \epsilon$ ) in  $L^2$ -norm (and expected rate  $2\sigma + \mu + 1/2 - \epsilon$  ( $1.1 - \epsilon$ ) in  $L^\infty$ -norm) rather than exponential convergence.

In Table 2, we observe that the relative errors decrease algebraically when we take  $\beta = \sigma + \mu - \lfloor \sigma + \mu \rfloor$ . Note that  $(1+x)^{-\sigma}f \in H^{5.5-\epsilon}(I)$ , and by Theorem 2.4, we have  $(1+x)^{-\sigma-\mu}u \in B_{\omega^{\mu,-\mu}}^{5.5+\mu-\epsilon}(I)$ . Then, by Theorem 2.8, we have the order of convergence  $5.5 + \mu - \epsilon$  in  $L^2$ -norm and expect the order of convergence  $5 + \mu - \epsilon$  in  $L^\infty$ -norm as observed here. When taking  $\beta = \mu$ , we cannot reach the singularity index of the solution:  $(1+x)^{-\mu}u \in B_{\omega^{\mu,-\mu}}^{2\sigma+\mu+1-\epsilon}(I)$ , by  $f \in H^{2\sigma+1-\epsilon}(I)$  and Theorem 2.4. Thus, we can only expect algebraic convergence with rate  $2\sigma + \mu + 1/2 - \epsilon$  ( $2.3 - \epsilon$ ) in  $L^\infty$ -norm rather than the order  $5 + \mu - \epsilon$ .

In Table 3,  $f$  is analytic, and by Theorem 2.4,  $(1+x)^{-\beta}u$  ( $\beta = \mu$ ) is infinitely smooth (analytic, to be precise). By Theorem 2.8, we obtain the exponential convergence.

*Example 4.2* (spectral collocation methods). Here, we test the spectral collocation method (2.16) using the formulation (2.19). In (1.1), we take  $u_0 = 0$ .

In all the numerical results presented here, we use  $\delta = \gamma = 0$  in (2.16). We also tested different cases of  $\delta, \gamma$  in the set  $\{-\mu, \mu, 0\}$ , and the numerical results are very similar: with the same number of nodes, we have same levels of accuracy.

In Table 4, we have similar observations as in Table 1 for spectral Petrov–Galerkin methods: taking  $\beta = \sigma + \mu - \lfloor \sigma + \mu \rfloor$  leads to better accuracy. We also observe that the collocation methods admit a bit worse accuracy than the spectral Petrov–Galerkin methods, but the errors are at the same magnitudes.

TABLE 4

Spectral collocation methods, Case I, relative  $L^\infty$  error:  $\mu = 0.2, \sigma = 0.2$ :  $\beta = \sigma + \mu - \lfloor \sigma + \mu \rfloor$  (left) and  $\beta = \mu$  (right).

# Nodes	$\varrho_\infty^r$	$\varrho_\infty^r$	Order
4	1.3557e-03	9.6747e-02	–
8	3.0582e-08	5.7640e-02	0.75
16	7.7475e-15	3.3236e-02	0.79
32	8.0124e-15	1.7078e-02	0.96
64	9.8003e-15	6.5880e-03	1.37

TABLE 5

Spectral collocation methods, Case II with  $\mu = 0.8, \sigma = 0.5$ , relative  $L^\infty$  error:  $\beta = \sigma + \mu - \lfloor \sigma + \mu \rfloor$  (left) and  $\beta = \mu$  (right).

# Nodes	$\varrho_\infty^r$	Order	$\varrho_\infty^r$	Order
4	1.2070e-01	–	1.2073e-01	–
8	7.5193e-04	7.33	6.4467e-03	4.23
16	9.0775e-06	6.37	8.8683e-04	2.86
32	1.5566e-07	5.87	1.4345e-04	2.63
64	2.7884e-09	5.80	2.2911e-05	2.65

TABLE 6

Spectral collocation methods, Case III, relative  $L^\infty$  error:  $\beta = \mu = 0.2$  (left) and  $\beta = \mu = 0.8$  (right).

# Nodes	$\varrho_\infty^r$	$\varrho_\infty^r$
4	4.1401e-03	6.4941e-04
8	1.6201e-07	1.4480e-08
16	8.0030e-15	3.2190e-14

In Table 5, we observe that the relative errors decrease with algebraic order when we take  $\beta = \sigma + \mu - \lfloor \sigma + \mu \rfloor$ . Note that  $(1 + x)^{-\sigma - \mu} u \in B_{\omega^{\mu, -\mu}}^{5.5 + \mu - \epsilon}(I)$ , and then by Theorem 2.9, we have the order of convergence  $5.5 + \mu - \epsilon$  in  $L^2$ -norm and expect  $5 + \mu - \epsilon$  in  $L^\infty$ -norm as observed here. When taking  $\beta = \mu$ , we have only  $(1 + x)^{-\mu} u \in B_{\omega^{\mu, -\mu}}^{2\sigma + \mu + 1 - \epsilon}(I)$ . Thus, we can only expect algebraic convergence with rate  $2\sigma + \mu + 1/2 - \epsilon$  in  $L^\infty$ -norm rather than the order  $5 + \mu - \epsilon$ . This is similar to the case of spectral Petrov–Galerkin methods.

In Table 6, we observe exponential convergence as predicted since  $f$  is analytic. This is similar to the case of spectral Petrov–Galerkin methods. However, the accuracy of the spectral collocation method is a bit lower than the spectral Petrov–Galerkin method in this example.

**4.2. Half line.** Now we test the spectral Petrov–Galerkin method (3.12) using numerical integration on the right-hand side with Case I :  $f = x^\sigma e^{-3x}$ ; Case II :  $f = |1 - x|^5 e^{-x}$ ; Case III:  $f = (1 + \sin(x))e^{-3x}$ ; Case IV:  $f = (1 + x)^{-5} \sin(1 + x)$ .

The error is measured in the following sense:

$$(4.2) \quad \varrho_2^r = \frac{\|u_{\text{ref}} - u_N\|_{\rho^{1, -\beta}}}{\|u_{\text{ref}}\|_{\rho^{1, -\beta}}},$$

where the reference solution  $u_{\text{ref}}$  is obtained with  $N = 128$  in (3.12).

In Table 7, we observe that the weighted error (4.2) decreases with algebraic order when we take  $\beta = \sigma + \mu - \lfloor \sigma + \mu \rfloor$  in the trial basis  $Z_N^\beta$ ; see (3.10). Note that  $x^{-\sigma} f = e^{-3x}$  is analytic, and by Theorem 3.17, we have the exponential convergence

TABLE 7

*Spectral Petrov–Galerkin on the half line, Case I with  $\sigma = 0.1$  and  $\mu = 0.1$ , weighted  $L^2$  error:  $\beta = \mu + \sigma$  (left);  $\beta = \mu$  (right).*

# Nodes	$e_2^f$	Order	$e_2^r$	Order
4	3.0172e-01	–	1.9500e-01	–
8	9.4875e-02	1.67	6.1907e-02	1.66
16	9.4692e-03	3.32	5.4457e-02	0.18
32	9.4752e-05	6.64	3.0055e-02	0.86
64	9.5099e-09	13.28	1.2215e-02	1.30
80	9.5272e-11	20.63	7.8592e-03	1.98

TABLE 8

*Spectral Petrov–Galerkin on the half line, Case II, weighted  $L^2$  error:  $\beta = \mu = 0.1$  (left) and  $\beta = \mu = 0.8$  (right).*

# Nodes	$e_2^f$	Order	$e_2^r$	Order
4	2.5878e-01	–	1.9678e-01	–
8	1.6600e-01	0.64	9.7834e-02	1.01
16	1.7915e-02	3.21	8.7095e-03	3.49
32	1.1479e-03	3.96	4.4959e-04	4.28
64	1.6764e-04	2.78	5.1485e-05	3.13

TABLE 9

*Spectral Petrov–Galerkin method on the half line, Case III, weighted  $L^2$  error:  $\beta = \mu = 0.1$  (left) and  $\beta = \mu = 0.8$  (right).*

# Nodes	$e_2^f$	Order	$e_2^r$	Order
4	1.7149e-01	–	1.0456e-01	–
8	2.7270e-02	2.65	1.3784e-02	2.92
16	2.6543e-03	3.36	1.0949e-03	3.65
32	2.9645e-05	6.48	9.7112e-06	6.82
64	3.5049e-08	9.72	9.0911e-09	10.06
80	1.4998e-10	24.44	3.6048e-11	24.78

TABLE 10

*Spectral Petrov–Galerkin method on the half line, Case IV, weighted  $L^2$  error:  $\beta = \mu = 0.1$  (left) and  $\beta = \mu = 0.8$  (right).*

# Nodes	$e_2^f$	Order	$e_2^r$	Order
4	3.7547e-01	–	2.5650e-01	–
8	1.5999e-01	1.23	8.8239e-02	1.54
16	3.7340e-02	2.10	1.6400e-02	2.43
32	3.4861e-03	3.42	1.2146e-03	3.76
64	8.5076e-05	5.36	2.3416e-05	5.70
80	1.7657e-05	7.05	4.5020e-06	7.39

as observed here. When taking  $\beta = \mu$ , we can only expect algebraic convergence with rate  $(\sigma + \mu + 1)/2 - \epsilon$  in the weighted  $L^2$ -norm, rather than exponential convergence.

In Table 8,  $f$  belongs to  $B_{\alpha,0}^r(\Lambda)$  with  $r = 5.5 - \epsilon$ . According to Theorem 3.3, the weighted  $L^2$  error is expected to be of order  $(r + \mu)/2 - \epsilon$ :  $2.8 - \epsilon$  when  $\mu = 0.1$ , and  $3.15 - \epsilon$  when  $\mu = 0.8$ .

We now test the cases of smooth right-hand side but with a different decay rate at infinity:  $f$  decays exponentially in Table 9 and  $f$  decays algebraically in Table 10. We observe spectral convergence in both tables but with different error behaviors.

When the solution decays exponentially at infinity ( $f = (1 + \sin(x))e^{-3x}$  decays exponentially), the weighted  $L^2$  errors decay faster than the case in Table 10, where the solution decays algebraically at infinity ( $f = (1 + x)^{-5} \sin(1 + x)$  decays algebraically). Here, the derivatives of  $u$  at infinity (and large value points) are much smaller when the solution decays faster at infinity. Thus, by Theorem 3.17, the weighted  $L^2$ -errors are smaller as the derivatives of  $u$  in the weighted  $L^2$ -norms are smaller, which is the case for fast decaying  $u$  at infinity.

**5. Proofs.**

**5.1. Proof of regularity.** To prove Theorem 2.2, we need the following lemma. Denote  $W^{\mu,p}$  as the standard Sobolev space ( $W^{\mu,2}(I) = H^\mu(I)$ ) and that

$$(5.1) \quad I_+^\mu(L^p(I)) = \{v|v = {}_{-1}\mathcal{I}_x^\mu \phi, \phi \in L^p(I)\}, \quad I_-^\mu(L^p(I)) = \{v|v = {}_x\mathcal{I}_1^\mu \phi, \phi \in L^p(I)\}.$$

LEMMA 5.1 (see [34, Theorem 18.3]). For  $0 < \mu < 1/p$  and  $1 < p < \infty$ ,

$$(5.2) \quad W^{\mu,p}(I) = I_+^\mu(L^p(I)) = I_-^\mu(L^p(I)).$$

When  $1/p < \mu < 1/p + 1$ ,

$$(5.3) \quad I_+^\mu(L^p(I)) = {}_0W^{\mu,p}(I), \quad {}_0W^{\mu,p}(I) = W^{\mu,p}(I) \cap \{v|v(-1) = 0\}.$$

Theorem 2.2 follows from Lemma 5.1 and the Sobolev embedding theorem; see, e.g., [1].  $\square$

*Proof of Proposition 2.3.* The conclusion for  $0 < \mu < 1/2$  follows readily from Lemma 5.1 or Lemma 2.5 in [28]. Now we prove the case for  $1/2 < \mu < 1$ . First, by Lemma 5.1 and (A.2), it holds that  ${}_0H^\mu(I) = I_+^\mu(L^2(I)) \subset J_L^\mu(I)$ . Next, we will prove that  $J_L^\mu(I) \subset {}_0H^\mu(I) \oplus \{(x + 1)^{\mu-1}\}$ . For any  $v \in J_L^\mu(I)$  (i.e.,  $v, {}_{-1}\mathcal{D}_x^\mu v \in L^2(I)$ ), we will show that  $v \in {}_0H^\mu(I)$ . We note that  ${}_{-1}\mathcal{I}_x^{1-\mu}v$  (to be precise, a version of  ${}_{-1}\mathcal{I}_x^{1-\mu}v$ ) is absolutely continuous, as it can be readily shown that  ${}_{-1}\mathcal{I}_x^{1-\mu}v \in H^1(I)$ . Then, by (A.4),

$$v - (x + 1)^{\mu-1} \lim_{x \rightarrow -1} {}_{-1}\mathcal{I}_x^{1-\mu}v / \Gamma(\mu) = {}_{-1}\mathcal{I}_x^\mu {}_{-1}\mathcal{D}_x^\mu v \in I_+^\mu(L^2(I)) = {}_0H^\mu(I).$$

This ends the proof of Proposition 2.3.  $\square$

*Remark 5.2.* Define the space  $J_R^\mu(I) = \{v|v, {}_x\mathcal{D}_1^\mu v \in L^2(I)\}$  equipped with the norm  $\|u\|_{J_R^\mu} = (\|{}_x\mathcal{D}_1^\mu u\|^2 + \|u\|^2)^{1/2}$ . Similarly, we have, denoting  ${}_0H^\mu(I) =: H^\mu(I) \cap \{v|v(1) = 0\}$ ,

$$J_R^\mu(I) = {}_0H^\mu(I) \oplus \{(1 - x)^{\mu-1}\}, \quad 1/2 < \mu < 1; \quad J_R^\mu(I) = H^\mu(I), \quad 0 < \mu < 1/2.$$

*Proof Theorem 2.4.* We first prove the conclusion for nonnegative integers  $r = k$ . For any positive real number  $r$ , the conclusion can be established by the space interpolation theory; see, e.g., [1]. Since  $\omega^{0,\mu-\beta}f \in B_{\omega^{\alpha,\beta-\mu}}^r(I)$  ( $r \geq 0$ ), we have  $f \in L_{\omega^{\alpha,\beta-\mu}}^2(I)$ . To assure the consistency condition (2.2), we have to identify the range of parameters  $\alpha, \beta - \mu$ . By the Cauchy–Schwarz inequality, we obtain

$$|{}_{-1}\mathcal{I}_x^\mu f|^2 \leq \frac{1}{[\Gamma(\mu)]^2} \int_{-1}^x [\omega^{0,\mu-\beta}f]^2 \omega^{\alpha,\beta-\mu} dx \int_{-1}^x \frac{\omega^{-\alpha,\beta-\mu}(y)}{(x - y)^{2-2\mu}} dy,$$

by which we require  $\beta > 1 - \mu$ , such that (2.2) holds (and thus (2.3)). When  $\omega^{0,\mu-\beta}f \in C(\bar{I})$ , it can be readily shown that (2.2) and (2.3) hold.

Write  $\omega^{0,\mu-\beta} f(x) = \sum_{n=0}^{\infty} \tilde{f}_n P_n^{\alpha,\beta-\mu}(x)$ . By (2.3), the Fubini theorem, and (B.4), we have

$$u = {}_{-1}\mathcal{I}_x^\mu f = \sum_{n=0}^{\infty} \tilde{f}_{n-1} \mathcal{I}_x^\mu [\omega^{0,\beta-\mu} P_n^{\alpha,\beta-\mu}] = \omega^{0,\beta} \sum_{n=1}^{\infty} \frac{\Gamma(n + \beta - \mu + 1)}{\Gamma(n + \beta + 1)} \tilde{f}_n P_n^{\alpha-\mu,\beta}(x).$$

By (B.2) and the fact (which can be proved by Stirling’s formula) that

$$(5.4) \quad \lim_{n \rightarrow \infty} \frac{\Gamma(n + \delta)}{n^{\delta-\gamma} \Gamma(n + \gamma)} = \lim_{n \rightarrow \infty} \left( 1 + \frac{(\delta - \gamma)(\delta + \gamma - 1)}{2n} + \mathcal{O}(n^{-2}) \right) = 1,$$

we obtain that there exists constants  $C_1, C_2$  independent of  $n$  such that

$$(5.5) \quad C_1 \|P_n^{\alpha-\mu,\beta}\|_{\omega^{\alpha-\mu,\beta}}^2 \leq \|P_n^{\alpha,\beta-\mu}\|_{\omega^{\alpha,\beta-\mu}}^2 \leq C_2 \|P_n^{\alpha-\mu,\beta}\|_{\omega^{\alpha-\mu,\beta}}^2, \quad \alpha - \mu, \beta > -1,$$

which we denote by  $\|P_n^{\alpha,\beta-\mu}\|_{\omega^{\alpha,\beta-\mu}}^2 \approx \|P_n^{\alpha-\mu,\beta}\|_{\omega^{\alpha-\mu,\beta}}^2$ . By (2.3), (B.1), and (5.5), we have

$$\begin{aligned} & \|\partial_x^k [\omega^{0,-\beta} u]\|_{\omega^{\alpha-\mu+k,\beta+k}}^2 \\ &= \left\| \partial_x^k \sum_{n=1}^{\infty} \frac{\Gamma(n + \beta - \mu + 1)}{\Gamma(n + \beta + 1)} \tilde{f}_n P_n^{\alpha-\mu,\beta} \right\|_{\omega^{\alpha-\mu+k,\beta+k}}^2 \\ &= \sum_{n=k}^{\infty} \tilde{f}_n^2 \left( \frac{\Gamma(n + \beta - \mu + 1)}{\Gamma(n + \beta + 1)} \right)^2 (d_{n,k}^{\alpha,\beta-\mu})^2 \|P_{n-k}^{\alpha-\mu+k,\beta+k}\|_{\omega^{\alpha-\mu+k,\beta+k}}^2 \\ &\approx \sum_{n=k}^{\infty} \tilde{f}_n^2 \left( \frac{\Gamma(n + \beta - \mu + 1)}{\Gamma(n + \beta + 1)} \right)^2 (d_{n,k}^{\alpha,\beta-\mu})^2 \|P_{n-k}^{\alpha+k,\beta-\mu+k}\|_{\omega^{\alpha+k,\beta-\mu+k}}^2 \\ (5.6) \quad &\approx \sum_{n=k}^{\infty} \tilde{f}_n^2 n^{-2\mu} (d_{n,k}^{\alpha,\beta-\mu})^2 \|P_{n-k}^{\alpha+k,\beta-\mu+k}\|_{\omega^{\alpha+k,\beta-\mu+k}}^2, \end{aligned}$$

where  $d_{n,k}^{\alpha,\beta-\mu} = \frac{\Gamma(n+k+\alpha+\beta-\mu+1)}{2^k \Gamma(n+\alpha+\beta-\mu+1)}$  and we have used (5.4). Recall that we have

$$\begin{aligned} \|\partial_x^k [\omega^{0,\mu-\beta} f]\|_{\omega^{\alpha+k,\beta-\mu+k}}^2 &= \left\| \partial_x^k \sum_{n=0}^{\infty} \tilde{f}_n P_n^{\alpha,\beta-\mu} \right\|_{\omega^{\alpha+k,\beta-\mu+k}}^2 \\ &= \left\| \sum_{n=k}^{\infty} \tilde{f}_n d_{n,k}^{\alpha,\beta-\mu} P_{n-k}^{\alpha+k,\beta-\mu+k} \right\|_{\omega^{\alpha+k,\beta-\mu+k}}^2 \\ (5.7) \quad &= \sum_{n=k}^{\infty} \tilde{f}_n^2 (d_{n,k}^{\alpha,\beta-\mu})^2 \|P_{n-k}^{\alpha+k,\beta-\mu+k}\|_{\omega^{\alpha+k,\beta-\mu+k}}^2. \end{aligned}$$

By (5.6) and (5.7), we reach the conclusion by the space interpolation theory.  $\square$

**5.2. Proof of fractional formula of integration by parts.** We need the following lemmas to prove Theorem 2.5.

LEMMA 5.3 (fractional integration by parts, [34, Corollary of Theorem 2.4]). *Suppose that  $f = {}_{-1}\mathcal{I}_x^\mu \phi$ ,  $\phi \in L^p(I)$ , and  $g = {}_x\mathcal{I}_1^\mu \psi$ ,  $\psi \in L^q(I)$ , where  $1/p + 1/q \leq 1 + \mu$  and  $p, q \geq 1$ . Then, for any  $0 < \mu < 1$ , it holds that*

$$(5.8) \quad ({}_{-1}\mathcal{D}_x^\mu f, g) = (f, {}_x\mathcal{D}_1^\mu g).$$

LEMMA 5.4. Suppose that  $f = {}_{-1}\mathcal{I}_x^\mu \phi$ ,  $\phi \in L^p(I)$ , and  $g = {}_x\mathcal{I}_1^{\mu_2} \psi$ ,  $\psi \in L^q(I)$ , where  $1/p + 1/q \leq 1 + \mu$  and  $p, q \geq 1$ . Then, for any  $0 < \mu < 1$ , it holds that

$$(5.9) \quad ({}_{-1}\mathcal{D}_x^\mu f, g) = ({}_x\mathcal{D}_1^{\mu_1} f, {}_x\mathcal{D}_1^{\mu_2} g),$$

where  $0 \leq \mu_1, \mu_2 \leq \mu$ , and  $\mu_1 + \mu_2 = \mu$ .

Lemma 5.4 follows readily from Lemma 5.3 and the following composition rule.

LEMMA 5.5 (composition rule, [34, Corollary of Theorem 2.5]). If  $v = I_+^\mu(L^1(I))$  (see (5.1)) and  $0 < \mu < 1$ , then for any  $\mu_1, \mu_2 \geq 0$  with  $\mu_1 + \mu_2 = \mu$ ,

$$(5.10) \quad {}_{-1}\mathcal{D}_x^{\mu_1} {}_{-1}\mathcal{D}_x^{\mu_2} v = {}_{-1}\mathcal{D}_x^\mu v.$$

By Lemmas 5.1 and 5.3, we will prove a special case of Theorem 2.5 with  $\mu_2 = \mu$ .

THEOREM 5.6. Suppose that  $0 < \mu < 1$ . For  $f \in H^\mu(I)$  and  $g \in H^\mu(I)$ , it holds that

$$(5.11) \quad ({}_{-1}\mathcal{D}_x^\mu f, g) = (f, {}_x\mathcal{D}_1^\mu g).$$

*Proof.* When  $0 < \mu \leq 1/2$ , (5.11) can be readily checked from Lemmas 5.1 and 5.3. When  $1/2 < \mu < 1$ , by Lemma 5.3, (5.11) holds for the following cases:

- (1)  $f - f(-1) \in {}_0H^\mu(I) = I_+^\mu(L^2(I))$  and  $g - g(1) \in {}_0H^\mu(I) = I_-^\mu(L^2(I))$  with  $p = q = 2$  ( $1/p + 1/q = 1 < 1 + \mu$ ).
- (2)  $f(-1) \in I_+^\mu(L^1(I))$  and  $g - g(1) \in {}_0H^\mu(I) = I_-^\mu(L^2(I))$  with  $p = 1$  and  $q = 2$  ( $1/p + 1/q = 3/2 < 1 + \mu$ ).
- (3)  $f - f(-1) \in {}_0H^\mu(I) = I_+^\mu(L^2(I))$  and  $g(1) \in I_-^\mu(L^1(I))$  with  $p = 2$  and  $q = 1$  ( $1/p + 1/q = 3/2 < 1 + \mu$ ).

Then we have

$$\begin{aligned} ({}_{-1}\mathcal{D}_x^\mu f, g) &= ({}_{-1}\mathcal{D}_x^\mu [f - f(-1)], g - g(1)) + ({}_{-1}\mathcal{D}_x^\mu f(-1), g - g(1)) \\ &\quad + ({}_{-1}\mathcal{D}_x^\mu [f - f(-1)], g(1)) + ({}_{-1}\mathcal{D}_x^\mu [f(-1)], g(1)) \\ &= (f - f(-1), {}_x\mathcal{D}_1^\mu [g - g(1)]) + (f(-1), {}_x\mathcal{D}_1^\mu [g - g(1)]) \\ &\quad + (f - f(-1), {}_x\mathcal{D}_1^\mu [g(1)]) + (f(-1), {}_x\mathcal{D}_1^\mu [g(1)]) \\ &= (f, {}_x\mathcal{D}_1^\mu g), \end{aligned}$$

where we also use the fact that  $({}_{-1}\mathcal{D}_x^\mu [f(-1)], g(1)) = ([f(-1)], {}_x\mathcal{D}_1^\mu [g(1)])$ . □

*Proof of Theorem 2.5.* By Theorem 5.6 and Lemma 5.5, we have

$$(5.12) \quad ({}_{-1}\mathcal{D}_x^\mu f, g) = ({}_{-1}\mathcal{D}_x^{\mu_2+\mu_1} f, g) = ({}_{-1}\mathcal{D}_x^{\mu_2} {}_{-1}\mathcal{D}_x^{\mu_1} f, g) = ({}_{-1}\mathcal{D}_x^{\mu_1} f, {}_x\mathcal{D}_1^{\mu_2} g),$$

where  $\mu_1, \mu_2 \geq 0$  and  $\mu = \mu_1 + \mu_2$ . This proves Theorem 2.5. □

**5.3. Proofs of error estimates on a finite interval.** We need the following Hardy inequality for optimal error estimates.

LEMMA 5.7. For any  $\phi = \sum_{n=N+1}^\infty \phi_n P_n^{\alpha, \beta - \mu}(x) \in L^2_{\alpha, \beta - \mu}(I)$ ,  $N \geq 1$  and  $\alpha, \beta > \mu - 1$ , and then for any  $0 \leq \mu_2 \leq \mu$ , there exists a constant  $C > 0$  independent of  $N$  such that

$$\|{}_{-1}\mathcal{I}_x^{\mu_2} [\omega^{0, \beta - \mu} \phi]\|_{\omega^{\alpha - \mu_2, -\beta + \mu_1}} \leq CN^{-\mu_2} \|\phi\|_{\omega^{\alpha, \beta - \mu}}, \quad \mu_1 = \mu - \mu_2.$$



*Proof.* We have by (B.4) and (5.4)

$$\begin{aligned} & \left\| {}_{-1}\mathcal{I}_x^{\mu_2} [\omega^{0,\beta-\mu} \phi] \right\|_{\omega^{\alpha-\mu_2, -\beta+\mu_1}}^2 \\ &= \left\| \omega^{0,\beta-\mu_1} \sum_{n=N+1}^{\infty} \phi_n \frac{\Gamma(n+\beta-\mu+1)}{\Gamma(n+\beta-\mu_1+1)} P_n^{\alpha-\mu_2, \beta-\mu_1} \right\|_{\omega^{\alpha-\mu_2, -\beta+\mu_1}}^2 \\ &\leq C \sum_{n=N+1}^{\infty} \phi_n^2 \left\| \frac{\Gamma(n+\beta-\mu+1)}{\Gamma(n+\beta-\mu_1+1)} P_n^{\alpha-\mu_2, \beta-\mu_1} \right\|_{\omega^{\alpha-\mu_2, \beta-\mu_1}}^2 \\ &\leq CN^{-2\mu_2} \sum_{n=N+1}^{\infty} \phi_n^2 \|P_n^{\alpha, \beta-\mu}\|_{\omega^{\alpha, \beta-\mu}}^2 \leq CN^{-2\mu_2} \|\phi\|_{\omega^{\alpha, \beta-\mu}}^2. \end{aligned}$$

In the last line, we also used the fact (5.5).  $\square$

**5.3.1. Proof of Theorem 2.8.** We need the following estimate of the  $L^2_{\omega^{\alpha, \beta}}$ -projection error.

**THEOREM 5.8** (projection error, [21, Theorem 2.1]). *For any  $v \in B^r_{\omega^{\alpha, \beta}}(I)$  and for all  $0 \leq r_1 \leq r$ ,*

$$(5.13) \quad \left\| \pi_N^{\alpha, \beta} v - v \right\|_{r_1, \omega^{\alpha, \beta}} \leq C(N(N + \alpha + \beta))^{\frac{r_1-r}{2}} |v|_{r, \omega^{\alpha, \beta}, B},$$

where  $C$  is a generic positive constant independent of any function  $v$ ,  $N$ ,  $\alpha$ ,  $\beta$ .

Let  $\mu_2 = \mu - \mu_1$ . Set  $v = {}_x\mathcal{I}_1^{\mu_2} [\omega^{\alpha-\mu_2, \mu_1-\beta}(x) {}_{-1}\mathcal{D}_x^{\mu_1} u_N]$ . It can be readily checked that  $v \in Y_N^\alpha$  and  ${}_x\mathcal{D}_1^{\mu_2} v = \omega^{\alpha-\mu_2, \mu_1-\beta}(x) {}_{-1}\mathcal{D}_x^{\mu_1} u_N$  as  $u_N \in X_N^\beta$ . Then we have, by (A.4) and Lemma A.1,

$$\begin{aligned} \left\| {}_{-1}\mathcal{D}_x^{\mu_1} u_N \right\|_{\omega^{\alpha-\mu_2, \mu_1-\beta}}^2 &= (\omega^{0,\beta-\mu} \pi_N^{\alpha, \beta-\mu} \tilde{f}, {}_x\mathcal{I}_1^{\mu_2} ({}_x\mathcal{D}_1^{\mu_2} v)) \\ &= ({}_{-1}\mathcal{I}_x^{\mu_2} [\omega^{0,\beta-\mu} \pi_N^{\alpha, \beta-\mu} \tilde{f}], {}_x\mathcal{D}_1^{\mu_2} v) \\ &\leq \left\| {}_{-1}\mathcal{I}_x^{\mu_2} [\omega^{0,\beta-\mu} \pi_N^{\alpha, \beta-\mu} \tilde{f}] \right\|_{\omega^{\alpha-\mu_2, \mu_1-\beta}} \left\| {}_{-1}\mathcal{D}_x^{\mu_1} u_N \right\|_{\omega^{\alpha-\mu_2, \mu_1-\beta}}, \end{aligned}$$

and thus the stability (2.20) holds.

To obtain the convergence rate, we estimate  $e_N =: u_N - u^*$ , where  $u^* \in X_N^\beta$  is defined by  $\omega^{0,\beta} \pi_N^{\alpha-\mu, \beta} [\omega^{0,-\beta} u]$ , and we can obtain the desired estimate by the triangle inequality. Denote  $\eta = u - u^*$ . Then, by (1.1), (2.10), and Theorem 2.5, we have

$$(5.14) \quad ({}_{-1}\mathcal{D}_x^{\mu_1} e_N, {}_x\mathcal{D}_1^{\mu_2} v) = (\omega^{0,\beta-\mu} [\pi_N^{\alpha, \beta-\mu} \tilde{f} - \tilde{f}], v) + ({}_{-1}\mathcal{D}_x^{\mu_1} \eta, {}_x\mathcal{D}_1^{\mu_2} v).$$

Taking  $v \in Y_N^\alpha$  such that  ${}_x\mathcal{D}_1^{\mu_2} v = \omega^{\alpha-\mu_2, \mu_1-\beta}(x) {}_{-1}\mathcal{D}_x^{\mu_1} e_N$ , we then have

$$\left\| {}_{-1}\mathcal{D}_x^{\mu_1} e_N \right\|_{\omega^{\alpha-\mu_2, \mu_1-\beta}}^2 = ({}_{-1}\mathcal{I}_x^{\mu_2} \omega^{0,\beta-\mu} [\pi_N^{\alpha, \beta-\mu} \tilde{f} - \tilde{f}], {}_{-1}\mathcal{D}_x^{\mu_2} v) + ({}_{-1}\mathcal{D}_x^{\mu_1} \eta, {}_x\mathcal{D}_1^{\mu_2} v),$$

and thus by Cauchy-Schwarz inequality and the fact that  $({}_{-1}\mathcal{D}_x^{\mu_1} \eta, {}_x\mathcal{D}_1^{\mu_2} v) = 0$ ,

$$(5.15) \quad \left\| {}_{-1}\mathcal{D}_x^{\mu_1} e_N \right\|_{\omega^{\alpha-\mu_2, \mu_1-\beta}} \leq \left\| {}_{-1}\mathcal{I}_x^{\mu_2} (\omega^{0,\beta-\mu} [\pi_N^{\alpha, \beta-\mu} \tilde{f} - \tilde{f}]) \right\|_{\omega^{\alpha-\mu_2, \mu_1-\beta}}.$$

By (5.15) and Lemma 5.7, we obtain

$$\begin{aligned} (5.16) \quad \left\| {}_{-1}\mathcal{D}_x^{\mu_1} e_N \right\|_{\omega^{\alpha-\mu_2, \mu_1-\beta}} &\leq CN^{-\mu_2} \left\| \omega^{0,\beta-\mu} [\pi_N^{\alpha, \beta-\mu} \tilde{f} - \tilde{f}] \right\|_{\omega^{\alpha, \mu-\beta}} \\ &\leq CN^{-\mu_2} \left\| \pi_N^{\alpha, \beta-\mu} \tilde{f} - \tilde{f} \right\|_{\omega^{\alpha, \beta-\mu}} \\ &\leq CN^{-r-\mu_2} \left\| \partial_x^r \tilde{f} \right\|_{\omega^{\alpha+r, \beta-\mu+r}}. \end{aligned}$$

We claim that  $\|_{-1}\mathcal{D}_x^{\mu_1}\eta\|_{\omega^{\alpha-\mu_2,\mu_1-\beta}} \leq CN^{-r-\mu_2}\|\partial_x^r\tilde{f}\|_{\omega^{\alpha+r,\beta-\mu+r}}$ . In fact, we have  $_{-1}\mathcal{D}_x^{\mu_1}\eta = _{-1}\mathcal{I}_x^{\mu_2}(\omega^{0,\beta-\mu}[\pi_N^{\alpha,\beta-\mu}\tilde{f} - \tilde{f}])$  since  $_{-1}\mathcal{D}_x^{\mu_1}u = _{-1}\mathcal{I}_x^{\mu_2} _{-1}\mathcal{D}_x^{\mu}u = _{-1}\mathcal{I}_x^{\mu_2}f$  and  $_{-1}\mathcal{D}_x^{\mu_1}u^* = _{-1}\mathcal{I}_x^{\mu_2}(\omega^{0,\beta-\mu}\pi_N^{\alpha,\beta-\mu}\tilde{f})$  by the definition of  $u^* = \omega^{0,\beta}\pi^{\alpha-\mu,\beta}[\omega^{0,-\beta}u]$  and (2.3). Then the desired claim follows from Lemma 5.7. We then have from the triangle inequality (using  $u_N - u = \eta + e_N$ ) that

$$\|_{-1}\mathcal{D}_x^{\mu_1}(u_N - u)\|_{\omega^{\alpha-\mu_2,\mu_1-\beta}} \leq CN^{-r-\mu_2}\|\partial_x^r\tilde{f}\|_{\omega^{\alpha+r,\beta-\mu+r}}.$$

This ends the proof of Theorem 2.8.  $\square$

**5.3.2. Proof of Theorem 2.9.** For the Gauss–Jacobi interpolation, we have the following optimal error estimate.

LEMMA 5.9 (interpolation error, [27, Theorem 3.2.1]). *Assuming that  $v \in B_{\omega^{\delta,\gamma}}^r(I)$  where  $r \geq 1$  and  $\delta, \gamma > -1$ , we have for  $\delta \leq \rho \leq \delta + 1$  and  $\gamma \leq \sigma \leq \gamma + 1$ ,*

$$(5.17) \quad \left\|(\mathcal{I}_N^{\delta,\gamma}v - v)\right\|_{\omega^{\rho,\sigma}} \leq CN^{-r}\|\partial_x^r v\|_{\omega^{\rho+r,\sigma+r}}, \quad 0 \leq l \leq r.$$

Now, we prove Theorem 2.9. We take fractional integral  $_{-1}\mathcal{I}_x^{\mu_2}$  ( $0 \leq \mu_2 = \mu - \mu_1 \leq \mu$ ) over both sides of (2.3), and then by (A.3), we have

$$(5.18) \quad _{-1}\mathcal{D}_x^{\mu_1}u_N = _{-1}\mathcal{D}_x^{\mu_1}[\mathcal{I}_{N,\beta}^{\delta,\gamma}u_N] = _{-1}\mathcal{I}_x^{\mu_2}[\mathcal{I}_{N,\beta-\mu}^{\delta,\gamma}f].$$

By (5.18), the numerical scheme (2.16) is stable in the following sense:

$$(5.19) \quad \|_{-1}\mathcal{D}_x^{\mu_1}u_N\|_{\omega^{\alpha,-\beta-\mu}} = \left\|_{-1}\mathcal{I}_x^{\mu_2}[\mathcal{I}_{N,\beta-\mu}^{\delta,\gamma}f]\right\|_{\omega^{\alpha,-\beta-\mu}}.$$

By (5.19) and Lemma 5.7, we have

$$\|_{-1}\mathcal{D}_x^{\mu_1}(u_N - u)\|_{\omega^{\alpha-\mu_2,-\beta+\mu_1}} \leq CN^{-\mu_2}\left\|\mathcal{I}_N^{\delta,\gamma}(\omega^{0,\mu-\beta}f) - \omega^{\alpha,\mu-\beta}f\right\|_{\omega^{\alpha,\beta-\mu}}.$$

Then, by Lemma 5.9, when  $-1 < \delta \leq \alpha \leq \delta + 1$  and  $-1 < \gamma \leq \beta - \mu \leq \gamma + 1$ , we obtain (2.22).  $\square$

**5.4. Proofs of error estimates on the half line.** To prove Lemma 3.2, we need the following formula of integration by parts.

LEMMA 5.10 (see [34, section 5.1]). *Suppose that  $f = {}_0\mathcal{I}_x^\mu\phi$ ,  $\phi \in L^p(\Lambda)$  and that  $g = {}_x\mathcal{I}_\infty^\mu\psi$ ,  $\psi \in L^q(\Lambda)$ , where  $1/p + 1/q = 1 + \mu$  and  $p, q > 1$ . Then, for any  $0 < \mu < 1$ , it holds that*

$$(5.20) \quad ({}_0\mathcal{D}_x^\mu f, g) = (f, {}_x\mathcal{D}_\infty^\mu g).$$

Lemma 3.2 follows readily from Lemma 5.10 and the composition rule that

$${}_0\mathcal{D}_x^{\mu_1}{}_0\mathcal{D}_x^{\mu-\mu_1}f = {}_0\mathcal{D}_x^\mu f, \quad 0 \leq \mu_1 \leq \mu \text{ for } x \in \Lambda \text{ and } f = {}_0\mathcal{I}_x^\mu\phi, \quad \phi \in L^p(\Lambda), \quad p \geq 1.$$

Actually, this composition rule is a ready corollary of Lemma 5.5.

We need the following Hardy inequality, but we omit the proof since the idea of the proof is similar to that of Lemma 5.7 for the case of finite interval.

LEMMA 5.11. *For  $\phi = \sum_{n=N+1}^\infty \phi_n L^{\alpha,\beta-\mu}(x) \in L_{\rho^{\alpha,\beta-\mu}}^2(\Lambda)$ ,  $N \geq 1$  and  $\beta - \mu > -1, \alpha > 0$ , and then for any  $0 \leq \mu_2 \leq \mu$ , there exists a constant  $C$  independent of  $N$  such that*

$$(5.21) \quad \|{}_0\mathcal{I}_x^{\mu_2}\phi\|_{\rho^{\alpha,\beta-\mu_2}} \leq C(\alpha N)^{-\mu_2/2}\|\phi\|_{\rho^{\alpha,\beta}}.$$

LEMMA 5.12 (projection error, [23, Theorem 2.1]). *For any  $v \in A_{\alpha,\beta}^r(\Lambda)$ , and any nonnegative integer  $r$ , there exists a constant  $C$  independent of  $N$  such that*

$$(5.22) \quad \left\| \Pi_N^{\alpha,\beta} v - v \right\|_{A_{\alpha,\beta}^\theta} \leq C(\alpha N)^{(\theta-r)/2} \|\partial_x^r v\|_{\rho^{\alpha,\beta+r}}, \quad 0 \leq \theta \leq \mu.$$

LEMMA 5.13 (interpolation error, [22, Theorem 3.5]). *For  $v \in A_{\alpha,\beta}^r(\Lambda) \cap A_{\alpha,\beta-1}^r(\Lambda)$  and an integer  $r \geq 1$ , there is a constant  $C > 0$  independent of  $N$  such that*

$$\begin{aligned} & \left\| \mathcal{I}_N^{\alpha,\beta} v - v \right\|_{\rho^{\alpha,\beta}} \\ & \leq C(\alpha N)^{(1-r)/2} (\alpha^{-1} \|\partial_x^r v\|_{\rho^{\alpha,\beta+r-1}} + (1 + \alpha^{-1/2})(\ln N)^{1/2} \|\partial_x^r v\|_{\rho^{\alpha,\beta+r}}). \end{aligned}$$

*Proof of Theorem 3.17.* Taking  $v_N \in \mathbb{P}_N(\Lambda)$  in the scheme (3.11) such that  ${}_x\mathcal{D}_\infty^{\mu_2}(v_N \rho^{\alpha,0}) = \rho^{\alpha,\mu_1-\beta} {}_0\mathcal{D}_x^{\mu_1} u_N$ , we then have

$$\|{}_0\mathcal{D}_x^{\mu_1} u_N\|_{\rho^{\alpha,\mu_1-\beta}}^2 = ({}_0\mathcal{I}_x^{\mu_2} f, {}_x\mathcal{D}_\infty^{\mu_2}(v_N \rho^{\alpha,0})) = ({}_0\mathcal{I}_x^{\mu_2} f, {}_0\mathcal{D}_x^{\mu_1} u_N)_{\rho^{\alpha,\mu_1-\beta}},$$

and thus

$$(5.23) \quad \|{}_0\mathcal{D}_x^{\mu_1} u_N\|_{\rho^{\alpha,\mu_1-\beta}} \leq \|{}_0\mathcal{I}_x^{\mu_2} f\|_{\rho^{\alpha,\mu_1-\beta}}.$$

To obtain the *convergence rate* of the scheme, we estimate  $e_N = u_N - u^*$ , where  $u^* = \rho^{0,\beta} \Pi_N^{\alpha,\beta} [\rho^{0,-\beta} u] \in Z_N^\beta$ . Then we obtained the desired estimate by the triangle inequality and the project error  $\eta = u^* - u$ .

By the definition of  $u^*$ , we have that  $({}_0\mathcal{D}_x^{\mu_1} \eta, {}_x\mathcal{D}_\infty^{\mu_2}[v_N \rho^{\alpha,0}]) = 0$  for any  $v \in P_N(\Lambda)$ . Thus, by (3.1), Lemma 3.2, and the scheme (3.11), we have

$$({}_0\mathcal{D}_x^{\mu_1} e_N, {}_x\mathcal{D}_\infty^{\mu_2}[v_N \rho^{\alpha,0}]) = (\rho^{0,\beta-\mu} (\Pi_N^{\alpha,\beta-\mu} [\rho^{0,\mu-\beta} f] - \rho^{0,\mu-\beta} f), v_N).$$

Taking  $v$  such that  ${}_x\mathcal{D}_\infty^{\mu_2}(v_N \rho^{\alpha,0}) = \rho^{\alpha,\mu_1-\beta} {}_0\mathcal{D}_x^{\mu_1} e_N$ , we then have

$$\|{}_0\mathcal{D}_x^{\mu_1} e_N\|_{\rho^{\alpha,\mu_1-\beta}}^2 = (\rho^{0,\beta-\mu} (\Pi_N^{\alpha,\beta-\mu} [\rho^{0,\mu-\beta} f] - \rho^{0,\mu-\beta} f), v_N),$$

and thus by the Cauchy-Schwarz inequality,

$$(5.24) \quad \|{}_0\mathcal{D}_x^{\mu_1} e_N\|_{\rho^{\alpha,\mu_1-\beta}} \leq \left\| {}_0\mathcal{I}_x^{\mu_2} (\rho^{0,\beta-\mu} (\Pi_N^{\alpha,\beta-\mu} [\rho^{0,\mu-\beta} f] - \rho^{0,\mu-\beta} f)) \right\|_{\rho^{\alpha,\mu_1-\beta}}.$$

By a similar argument in the proof of Lemma 5.7, we have

$$\begin{aligned} \|{}_0\mathcal{D}_x^{\mu_1} e_N\|_{\rho^{\alpha,\mu_1-\beta}} & \leq \left\| {}_0\mathcal{I}_x^{\mu_2} (\rho^{0,\beta-\mu} (\Pi_N^{\alpha,\beta-\mu} [\rho^{0,\mu-\beta} f] - \rho^{0,\mu-\beta} f)) \right\|_{\rho^{\alpha,\mu_1-\beta}} \\ & \leq C(\alpha N)^{-\mu_2/2} \left\| \Pi_N^{\alpha-\mu,\beta} [\rho^{0,\mu-\beta} f] - [\rho^{0,\mu-\beta} f] \right\|_{\rho^{\alpha,\beta-\mu}} \\ & \leq C(\alpha N)^{-(r+\mu_2)/2} \|\partial_x^r (\rho^{0,\mu-\beta} f)\|_{\rho^{\alpha,\beta-\mu+r}}. \end{aligned}$$

Similar to the proof in Theorem 2.8, we have

$$\|{}_0\mathcal{D}_x^{\mu_1} \eta\|_{\rho^{\alpha,\mu_1-\beta}} \leq C(\alpha N)^{-(r+\mu_2)/2} \|\partial_x^r (\rho^{0,\mu-\beta} f)\|_{\rho^{\alpha,\beta-\mu+r}}.$$

We then reach the conclusion by (5.24), Lemma 5.12, and the triangle inequality.  $\square$

*Proof of Theorem 3.4.* By (3.2) and (3.14), we have

$$u_N - u = -{}_1\mathcal{I}_x^\mu [\mathcal{I}_{N,\beta-\mu}^{\alpha,\gamma} f - f].$$

By Lemma 5.11, we have

$$(5.25) \quad \|u_N - u\|_{\rho^{\alpha,-\beta}} \leq C(\alpha N)^{-\mu/2} \|\mathcal{I}_N^{\alpha,\gamma} (\rho^{0,\mu-\beta} f) - \rho^{0,\mu-\beta} f\|_{\rho^{\alpha,\mu-\beta}}^2.$$

Then, by Lemma 5.13 for  $\gamma = \beta - \mu$ , we have (3.18).  $\square$

**6. Conclusion and discussion.** We have analyzed spectral Petrov–Galerkin/Galerkin and collocation methods for single-term Riemann–Liouville fractional ordinary differential equations. For this type of equation on the finite interval, the singularity of the solutions is of type  $(x - a)^\beta$ , where  $a$  is the left endpoint, and  $\beta$  is singularity index  $0 \leq \beta \leq 1$ ; when  $\beta = 0, 1$ , there is no singularity. This type of singularity can be well resolved with weighted Jacobi polynomials, i.e.,  $(x - a)^\beta$  times some linear combination of Jacobi polynomials. For equations on the half line, we can resolve the left endpoint boundary in a similar fashion when we know the decay rate of the solutions at infinity. In this work, we use generalized Laguerre polynomials. We note that better resolution at infinity may result from better knowledge of the decay behavior of the solution at infinity. In summary, for equations on both finite intervals and the half line, we recover the spectral convergence, as both error estimates and numerical results show.

Our methodology and analysis can be extended in several directions. First, we can extend to FODEs in a more general form, e.g.,

$$\frac{d}{dx}(a(x) {}_{-1}\mathcal{D}_x^\mu u) + c(x)u = f,$$

where  $a(x) > 0$  and  $c(x)$  are continuous and homogeneous Dirichlet boundary conditions are imposed. When  $c(x) = 0$ , see, e.g., [40], the extension of our analysis is more or less straightforward. When  $c(x) \neq 0$ , our analysis can be readily applied when the singular basis (2.9) with negative index is used, where we find that the numerical results are more accurate than those with positive index in (2.9). Second, we can extend the methodology presented here to high-dimensional problems on smooth domains as it is known that the singularity of high-dimensional problems may simply lie along the boundary; see, e.g., [39]. These two directions of research are ongoing.

**Appendix A. Properties of fractional integrals and derivatives.** We have used the following properties of Riemann–Liouville derivatives in this work:

- For  $0 < \mu < 1$ , we have, see, e.g., [20, (1.23)],

$$(A.1) \quad {}_{-1}\mathcal{D}_x^\mu v = 0 \Leftrightarrow v = c(x + 1)^{\mu-1},$$

where  $c$  is an arbitrary constant.

- (inverse, see, e.g., [34, Theorem 2.4], [20, (1.14)])

$$(A.2) \quad {}_{-1}\mathcal{D}_x^\mu {}_{-1}\mathcal{I}_x^\mu \phi = \phi \quad \text{for any } \phi \in L^1(I).$$

- (inverse, see, e.g., [34, Theorem 2.4]) If there exists an  $\phi \in L^1(I)$  such that  $f = {}_{-1}\mathcal{I}_x^\mu \phi$ , then

$$(A.3) \quad {}_{-1}\mathcal{I}_x^\mu {}_{-1}\mathcal{D}_x^\mu f = f.$$

However, if we assume only that  $f \in L^1(I)$  and  ${}_{-1}\mathcal{I}_x^{1-\mu} f$  is absolute continuous, then

$$(A.4) \quad {}_{-1}\mathcal{I}_x^\mu {}_{-1}\mathcal{D}_x^\mu f = f - (x + 1)^{\mu-1} \lim_{x \rightarrow -1} {}_{-1}\mathcal{I}_x^{1-\mu} f / \Gamma(\mu).$$

LEMMA A.1 (fractional integration by parts I, [34, Corollary of Theorem 3.5]).  
If  $\phi(x) \in L^p(I)$  and  $\psi(x) \in L^q(I)$ ,  $p, q \geq 1$ , we have

$$(A.5) \quad ({}_{-1}\mathcal{I}_x^\mu \phi, \psi) = (\phi, {}_x\mathcal{I}_1^\mu \psi),$$

where  $1/p + 1/q = 1 + \mu$  ( $p, q > 1$ ) or  $1/p + 1/q < 1 + \mu$ .

**Appendix B. Some useful relations of Jacobi polynomials.** The following relations hold for Jacobi polynomials, see, e.g., [4, Chapter 2]:

$$(B.1) \quad \partial_x P_n^{\alpha,\beta}(x) = \frac{n + \alpha + \beta + 1}{2} P_{n-1}^{\alpha+1,\beta+1}(x), \quad \alpha, \beta > -1.$$

$$(B.2) \quad \|P_n^{\alpha,\beta}\|_{\omega^{\alpha,\beta}}^2 = \frac{2^{\alpha+\beta+1}}{2n + \alpha + \beta + 1} \frac{\Gamma(n + \alpha + 1)\Gamma(n + \beta + 1)}{n!\Gamma(n + \alpha + \beta + 1)}, \quad \alpha, \beta > -1.$$

By (B.2) and (B.1), we have

$$(B.3) \quad \|P_n^{\alpha,\beta}\|_{\omega^{\alpha,\beta}}^2 = \frac{1}{(n + \alpha + \beta + 1)n} \|P_{n-1}^{\alpha+1,\beta+1}\|_{\omega^{\alpha+1,\beta+1}}^2.$$

The fractional integral of the weighted Jacobi polynomial is

$$(B.4) \quad {}_{-1}^{RL}\mathcal{I}_x^\mu((1+x)^\beta P_n^{\alpha,\beta}(x)) = \frac{\Gamma(n + \beta + 1)}{\Gamma(n + \beta + \mu + 1)} (1+x)^{\beta+\mu} P_n^{\alpha-\mu,\beta+\mu}(x),$$

where  $\alpha - 1 + \mu > -1$  and  $\beta - \mu + 1 > 0$ ; see, e.g., [4, (3.6)]. By the inverse property (A.2), we then have the fractional derivative of weighted Jacobi polynomials with  $\beta - \mu, \alpha > -1$ :

$$(B.5) \quad {}_{-1}\mathcal{D}_x^\mu((1+x)^\beta P_n^{\alpha,\beta}(x)) = \frac{\Gamma(n + \beta + 1)}{\Gamma(n + \beta - \mu + 1)} (1+x)^{\beta-\mu} P_n^{\alpha+\mu,\beta-\mu}(x).$$

Similarly, we have, for  $\alpha - \mu, \beta > -1$ ,

$$(B.6) \quad {}_x\mathcal{D}_1^\mu((1-x)^\alpha P_n^{\alpha,\beta}(x)) = \frac{\Gamma(n + \alpha + 1)}{\Gamma(n + \alpha - \mu + 1)} (1-x)^{\alpha-\mu} P_n^{\alpha-\mu,\beta+\mu}(x).$$

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