

# Spectral Methods for Substantial Fractional Differential Equations

Can Huang<sup>1</sup> · Zhimin Zhang<sup>2,3</sup> · Qingshuo Song<sup>4</sup>

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**Abstract** In this paper, a non-polynomial spectral Petrov–Galerkin method and its associated collocation method for substantial fractional differential equations are proposed, analyzed, and tested. We modify a class of generalized Laguerre polynomials to form our trial basis and test basis. After a proper scaling of these bases, our Petrov–Galerkin method results in diagonal and well-conditioned linear systems for certain types of fractional differential equations. In the meantime, we provide superconvergence points of the Petrov–Galerkin approximation for associated fractional derivative and function value of true solution. Additionally, we present explicit fractional differential collocation matrices based upon Laguerre–Gauss–Radau points. It is noteworthy that the proposed methods allow us to adjust a parameter in the basis according to different given data to maximize the convergence rate. All these findings have been proved rigorously in our convergence analysis and confirmed in our numerical experiments.

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✉ Can Huang  
canhuang@xmu.edu.cn

Zhimin Zhang  
zmzhang@csrc.ac.cn, zzhang@math.wayne.edu

Qingshuo Song  
qingsong@cityu.edu.hk

<sup>1</sup> School of Mathematical Science and Fujian Provincial Key Laboratory on Mathematical Modeling & High Performance Scientific Computing, Xiamen University, Fujian 361005, China

<sup>2</sup> Beijing Computational Science Research Center, Beijing 100094, China

<sup>3</sup> Department of Mathematics, Wayne State University, Detroit, MI 48202, USA

<sup>4</sup> Department of Mathematics, City University of Hong Kong, Kowloon, Hong Kong

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## 1 Introduction

With the development of advanced experimental technology, more and more particle diffusion processes in complex systems are revealed to follow anomalous diffusion instead of the traditional Gaussian statistics. These processes are characterized by deviations from traditional linear time dependence in their second moment  $\langle X(t) \rangle \sim t^\alpha$ ,  $\alpha \neq 1$ . In particular, these processes ( $0 < \alpha < 1$ ) have been a focal point in both physics and mathematics by virtue of their intrinsic connection with fractional differential equations (FDEs). This class of process has either infinite mean of waiting time or diverging jump length variance (Lévy flights). As a result, a general continuous time random walk (CTRW), rather than a Brownian motion, seems to be more competitive to model the anomalous diffusion of particles in a complex system [20] and this fact has been exploited in many applications such as underground environment problem [11], fluid flow [13], and turbulence and chaos [23]. Regarding their associated probability density functions, the CTRW with diverging mean of waiting time results in a Fokker–Planck equation (FPE) with fractional derivative in time whereas Lévy flights lead to a FPE with spatial fractional derivative [16].

Based upon an extension of CTRW to position-velocity space, Fredrich et al [8] generalized the standard concept of fractional derivative to a substantial fractional derivative as follows:

$$D_s^{\sigma, \nu} f(x) = \frac{1}{\Gamma(\nu)} \left[ \frac{d}{dx} + \sigma \right] \int_0^x (x-\tau)^{\nu-1} e^{-\sigma(x-\tau)} f(\tau) d\tau, \quad 0 < \nu < 1, \sigma > 0, x \in [0, \infty), \quad (1)$$

which has been intensively investigated in [3, 6, 28] and references therein. Recently, Chen and Deng et al [4] extended the definition to any order of  $\nu > 0$ . In this work, we shall adopt the definition in [4] and propose a non-polynomial spectral Petrov–Galerkin (PG) method and its associated collocation method for substantial fractional differential equations (FDEs).

As is well-known, by allowing trial space and test space to be different, the PG method has a remarkable advantage over the Galerkin method by choosing suitable test space to enhance computational efficiency while preserving its convergence order. By a careful selection of these two spaces, Karniadakis et al [32] obtained an explicit expression of their approximation (without solving a linear system) for certain Riemann–Liouville FDEs (RLFDEs). See [5, 12] for more references.

On the other hand, the spectral collocation method seeks a representation of the solution in terms of a finite-dimensional interpolant and a closure approximation based on setting equal to zero the residual at collocation points. For standard integer-order problems, interested readers are referred to [2, 24, 27]. Spectral collocation matrices for Riemann–Liouville fractional derivative are first proposed by Karniadakis et al [31] on the basis of “poly-factonomial” approximation, which is of the form  $\{(x+1)^\mu P_n^{\alpha, \beta}(x)\}_{n=0}^N$ , where  $P_n^{\alpha, \beta}(x)$ ,  $\alpha, \beta > -1$  is the Jacobi polynomial. For finite difference methods and finite element methods for traditional FDEs or FPDEs, readers are referred to [5, 7, 14, 18, 19, 22, 26, 29, 30, 32].

Compared with the extensive numerical methods developed for standard FDEs, the development of numerical schemes for substantial FDE is limited because of the relative newness of this field. As far as we know, numerical methods for substantial FDEs are predominately

finite difference methods (FDM) and particle tracking methods [1]. In [17], a comparative study of numerical solutions of three fractional partial differential equations in the framework of the class of Lévy models with substantial fractional derivative is explored. Recently, a high order finite difference scheme, namely, the tempered weighted and shifted Grünwald difference, for substantial FDE is provided in [15]. In contrast, spectral methods for substantial FDE have not been investigated and this work seems to be the first attempt in this direction.

It is worth emphasizing that we have derived, for the first time, identity (4) for substantial fractional derivatives. This identity is a counterpart of the Bateman fractional integral formula in Riemann–Liouville fractional derivatives. It plays an essential role in analyzing substantial fractional differential equations as the Bateman fractional integral formula does in [5, 31, 32] among others, for traditional fractional differential equations. Identity (4) provides a useful tool for further study on the subject and stands on its own as an important contribution. Based on this identity, our essential idea is to find a suitable basis of specific order of each equation which incorporates the initial condition(s) automatically and has an explicit expression of the required substantial fractional derivative. In particular, our method has the following prominent features:

- (1) Our basis consists of a combination of Laguerre polynomials  $L_n^\alpha(x)$ , exponential function  $e^{-\sigma x}$ , and power function  $x^\alpha$ . Hence, our method is far from a polynomial approximation.
- (2) By a careful selection of trial space and test space, our Petrov–Galerkin method yields a diagonal and well-conditioned linear system for each of our model problems.
- (3) In view of a priori known regularity of given data, we are able to adjust a parameter in our basis to achieve high order accuracy. Therefore, convergence rate can be enhanced for some specific choice of parameters.
- (4) We solve substantial FDEs on a semi-infinite domain without any domain truncation.

We point out that for standard RLFDE, PG methods and spectral collocation methods have been proposed in [5, 31, 32] within the framework of “Generalized Jacobi Function” approximation. In particular, a rigorous convergence analysis of PG methods is included in [5, 12]. However, our methods are essentially distinct from theirs. Firstly, the domain of substantial FDE is extended from  $[-1, 1]$  to  $[0, \infty)$ , which makes the numerical treatment more challenging. As will be shown later, our basis is neither “poly-factonomial” [32] nor “Generalized Jacobi Function” [5], but “modified Laguerre function”; Secondly, our spectral collocation matrices are completely explicit. The key is to provide a closed form of conversion from Lagrange interpolation polynomial to generalized Laguerre polynomials  $L_n^\lambda(x)$ ; Finally, the superconvergence points of our PG method are explored.

The rest of the paper is organized as follows. In Sect. 2, we shall recall some preliminary knowledge on generalized Laguerre polynomials/modified Laguerre functions. Some essential identities pertinent to our algorithms shall be introduced/derived. Then in Sect. 3, we shall explore a PG method for substantial FDEs. A convergence analysis will be provided. In Sect. 4, we shall present explicit spectral collocation algorithms and their convergence analysis. Finally, in Sect. 5, we shall study superconvergence properties of our PG method. All theoretical results are confirmed by associated numerical experiments.

## 2 Preliminary

In this section, we introduce some preliminary knowledge that will be used throughout the paper. In this work, we adopt the definition of substantial fractional derivative in [4, 8]. Let  $\mu, \sigma > 0$  and  $\mu \in [m - 1, m)$ , then

$$D_s^{\sigma, \mu} f(x) = \frac{1}{\Gamma(m - \mu)} D_s^m \left[ \int_0^x (x - \tau)^{m - \mu - 1} e^{-\sigma(x - \tau)} f(\tau) d\tau \right], x \in [0, \infty) \quad (2)$$

where

$$D_s^m = \left( \frac{d}{dx} + \sigma \right)^m = \underbrace{(D + \sigma) \cdots (D + \sigma)}_{m \text{ times}}, \quad D = \frac{d}{dx}.$$

## 2.1 Modified Laguerre Function

Associated with the definition of substantial fractional derivative (2), we define modified Laguerre functions by

$$\hat{L}_n^{\lambda, \sigma}(x) = x^\lambda e^{-\sigma x} L_n^\lambda(2\sigma x), \quad x \in [0, \infty), \quad n = 0, 1, \dots,$$

where  $\lambda \geq 0$ ,  $\sigma$  is a constant inherited from (2) and  $L_n^\lambda(y)$  is the standard generalized Laguerre polynomial. It is noteworthy that the generalized Laguerre function defined in [24, p. 241] is a special case of our definition.

Obviously, the modified Laguerre Function satisfies the three-term recurrence relation

$$\begin{cases} \hat{L}_0^{\lambda, \sigma}(x) = x^\lambda e^{-\sigma x}, \quad \hat{L}_1^{\lambda, \sigma}(x) = x^\lambda e^{-\sigma x} (-2\sigma x + \lambda + 1), \\ (n+1) \hat{L}_{n+1}^{\lambda, \sigma}(x) = (2n + \lambda + 1 - 2\sigma x) \hat{L}_n^{\lambda, \sigma}(x) - (n + \lambda) \hat{L}_{n-1}^{\lambda, \sigma}(x). \end{cases}$$

and the orthogonality

$$\int_0^\infty x^{-\lambda} \hat{L}_n^{\lambda, \sigma}(x) \hat{L}_m^{\lambda, \sigma}(x) dx = \left( \frac{1}{2\sigma} \right)^{1+\lambda} \frac{\Gamma(n + \lambda + 1)}{n!} \delta_{nm}. \quad (3)$$

Furthermore, it owns the following crucial property.

**Lemma 1** For any  $0 < \nu < 1$  and  $m = 1, 2, \dots$ , then

$$D_s^{m-\nu} \hat{L}_n^{\lambda, \sigma}(x) = \frac{\Gamma(\lambda + n + 1)}{\Gamma(\nu + \lambda + n - m + 1)} \hat{L}_n^{\lambda + \nu - m, \sigma}(x), \quad x \in [0, \infty) \quad (4)$$

provided  $\lambda + \nu - m \geq 0$ .

*Proof* We shall prove by induction and use the following identity [21, p.462]

$$\begin{aligned} \int_0^a (a-x)^{\beta-1} x^{\alpha-1} L_n^\lambda(cx) dx &= \frac{a^{\alpha+\beta-1} (\lambda+1)_n}{n!} B(\alpha, \beta) {}_2F_2 \\ &(-n, \alpha; \alpha+\beta, \lambda+1; ac), \quad \alpha, \beta > 0, \end{aligned} \quad (5)$$

where  $B(\cdot, \cdot)$  is the beta function and  ${}_pF_q(\cdot)$  is the standard hypergeometric function with parameters  $p$  and  $q$ . In particular, choosing  $\alpha = \lambda + 1$  in (5), and noting that  $L_n^\lambda(x) = \frac{\Gamma(n + \lambda + 1)}{\Gamma(n + 1)} {}_1F_1(-n; \lambda + 1; x)$ , one obtains

$$\int_0^a (a-x)^{\beta-1} x^\lambda L_n^\lambda(cx) dx = a^{\beta+\lambda} B(\beta, \lambda + n + 1) L_n^{\beta+\lambda}(ac),$$

which immediately implies

$$\int_0^x (x-\tau)^{\nu-1} e^{-\sigma(x-\tau)} \hat{L}_n^\lambda(\tau) d\tau = B(\nu, \lambda + n + 1) \hat{L}_n^{\nu+\lambda, \sigma}(x).$$

Therefore,

$$\begin{aligned}
 D_s^{\sigma, 1-\nu} \left[ \hat{L}_n^{\lambda, \sigma}(x) \right] &= \frac{\Gamma(\lambda + n + 1)}{\Gamma(\nu + \lambda + n + 1)} x^{\lambda+\nu-1} e^{-\sigma x} \left[ (\nu + \lambda) L_n^{\lambda+\nu}(2\sigma x) - 2\sigma x L_{n-1}^{\lambda+\nu+1}(2\sigma x) \right] \\
 &= \frac{\Gamma(\lambda + n + 1)}{\Gamma(\nu + \lambda + n + 1)} x^{\lambda+\nu-1} e^{-\sigma x} (n + \lambda + \nu) L_n^{\lambda+\nu-1}(2\sigma x) \\
 &= \frac{\Gamma(\lambda + n + 1)}{\Gamma(\nu + \lambda + n)} \hat{L}_n^{\lambda+\nu-1, \sigma}(x),
 \end{aligned} \tag{6}$$

where the following properties of standard Laguerre polynomials are used.

$$\begin{cases} \frac{d^k}{dx^k} L_n^\lambda(x) = (-1)^k L_{n-k}^{\lambda+k}(x), \\ x L_{n-1}^{\lambda+1}(x) = (n + \lambda) L_{n-1}^\lambda(x) - n L_n^\lambda(x), \\ L_n^\lambda(x) = L_n^{\lambda+1}(x) - L_{n-1}^{\lambda+1}(x). \end{cases}$$

Hence, (4) is true for  $m = 1$ . Suppose that it is true for  $m = k$ , then for  $m = k + 1$ , following the same fashion as (6), one easily obtains

$$\begin{aligned}
 D_s^{\sigma, k+1-\nu} \hat{L}_n^{\lambda, \sigma}(x) &= \left( \frac{d}{dx} + \sigma \right) D_s^{\sigma, k-\nu} \hat{L}_n^{\lambda, \sigma}(x) \\
 &= \frac{\Gamma(\lambda + n + 1)}{\Gamma(\nu + \lambda + n - k + 1)} \left( \frac{d}{dx} + \sigma \right) \hat{L}_n^{\lambda+\nu-k, \sigma}(x) \\
 &= \frac{\Gamma(\lambda + n + 1)}{\Gamma(\nu + \lambda + n - k)} \hat{L}_n^{\lambda+\nu-k-1, \sigma}(x).
 \end{aligned}$$

We are done.  $\square$

Note that if  $\lambda = 0$ , the substantial fractional derivative operator  $D_s^{\sigma, m-\nu}$  takes smooth functions  $e^{-\sigma x} L_n^0(2\sigma x)$  to  $\hat{L}_n^{\nu-m, \sigma}(x)$ . Conversely, if  $\lambda = m - \nu$ ,  $D_s^{\sigma, m-\nu}$  takes  $\hat{L}_n^{\lambda, \sigma}(x)$  to  $e^{-\sigma x} L_n^0(2\sigma x)$ . Such remarkable properties are essential for our algorithms.

## 2.2 Weighted Hilbert Space

Next, we introduce a space [9, 24] for the sake of analysis

$$B_{w^\alpha}^r([0, \infty)) = \{u \text{ is measurable and } \|u\|_{r, w^\alpha} < \infty\}$$

equipped with norm

$$\|u\|_{r, w^\alpha} = \left( \sum_{k=0}^r \|\partial_x^k u\|_{w^{\alpha+k}}^2 \right)^{1/2}$$

and the weight  $w^\alpha(x) = x^\alpha e^{-2\sigma x}$ . Consider the orthogonal projection  $\Pi_N^\alpha : B_{w^\alpha}^r \rightarrow P_N$  such that

$$(u - \Pi_N^\alpha u, v)_{w^\alpha} = 0, \quad \forall v \in P_N.$$

**Lemma 2** For any  $u \in B_{w^\alpha}^r$ ,  $m \leq r$ , there exists a constant  $C$  independent of  $N$  such that

$$\|\partial_x^m (u - \Pi_N^\alpha u)\|_{w^{\alpha+m}} \leq C N^{(m-r)/2} \|\partial_x^r u\|_{w^{\alpha+r}}.$$

*Proof* The result is a direct consequence of [24, Theorem 7.8] by making a change of variable  $y = 2\sigma x$ .  $\square$

### 2.3 Laguerre–Gauss–Radau Quadrature

For  $\lambda \geq 0$ , let  $\{x_i := x_{N,i}^{(\lambda)}, w_i := w_{N,i}^{(\lambda)}\}_{i=0}^N$  be the set of Laguerre–Gauss–Radau quadrature points and weights associated with  $\omega^\lambda(x) = x^\lambda e^{-2\sigma x}$ . Hereafter, we assume that  $\{x_i\}_{i=0}^N$  are arranged in ascending order so that  $x_0 = 0$ . Then  $\{x_i, w_i\}_{i=0}^N$  have the explicit expression [24, p. 243]

$$\begin{cases} x_0 = 0, \text{ and } \{x_i\}_{i=1}^N \text{ are zeros of } L_N^{1+\lambda}(2\sigma x). \\ w_0 = \frac{(\lambda+1)\Gamma^2(\lambda+1)N!}{\Gamma(N+\lambda+2)} \left(\frac{1}{2\sigma}\right)^{1+\lambda} \\ w_i = \frac{\Gamma(N+\lambda+1)}{N!(N+\lambda+1)} \frac{1}{[L_N^\lambda(2\sigma x_i)]^2} \left(\frac{1}{2\sigma}\right)^{1+\lambda}, 1 \leq i \leq N \end{cases}$$

and enjoys the exactness

$$\int_0^\infty p(x) x^\lambda e^{-2\sigma x} dx = \sum_{i=0}^N w_i p(x_i), \quad \forall p \in P_{2N}.$$

### 3 Petrov–Galerkin Method

In this section, we shall develop PG algorithms for substantial FDE based upon Lemma 1 and show that by choosing suitable trial space and test space, substantial fractional derivative operator can be discretized as a diagonal matrix. Similar property for standard Riemann–Liouville FDE has been exploited in [5, 12, 32].

To have more insight, we shall consider  $(m - \nu)$ ,  $m = 1$  or  $2$ ,  $0 < \nu < 1$  order problems just as [32] and [31].

#### 3.1 Substantial $(1 - \nu)$ Order FDE

We seek the approximation of solution to the simplest substantial FDE

$$\begin{cases} D_s^{\sigma, 1-\nu} u(x) = f(x), \quad 0 < \nu < 1, x \in (0, \infty) \\ u(0) = 0, \end{cases} \quad (7)$$

Motivated by (4), we establish our variational form in the trial space  $U_1^N = \text{span}\{(n+1)^{-\frac{\lambda-\nu+1}{2}} \hat{L}_n^{\lambda, \sigma}(x)\}_{n=0}^N$  and test space  $V_1^N = \text{span}\{(n+1)^{-\frac{\lambda+\nu-1}{2}} \hat{L}_n^{\lambda+\nu-1, \sigma}(x)\}_{n=0}^N$  with respect to the weight  $\hat{w}(x) = x^{1-\lambda-\nu}$ . Therefore, our Petrov–Galerkin scheme is to find  $u_N \in U_1^N$  with  $u_N(0) = 0$  such that

$$(D_s^{\sigma, 1-\nu} u_N, v)_{\hat{w}} = (f, v)_{\hat{w}}, \quad \forall v \in V_1^N.$$

In particular, we take the form

$$u_N(x) := \sum_{k=0}^N \frac{c_k}{(k+1)^{(\lambda-\nu+1)/2}} \hat{L}_k^{\lambda, \sigma}(x), \quad (8)$$

where  $c'_k$ s are coefficients to be determined. Applying (4) and (3), we obtain for  $0 \leq n \leq N$

$$\begin{aligned} & \left( f, \frac{1}{(1+n)^{(\lambda+\nu-1)/2}} \hat{L}_n^{\lambda+\nu-1, \sigma} \right)_{\hat{w}} \\ &= \sum_{k=0}^N \frac{c_k}{(1+n)^{(\lambda+\nu-1)/2} (k+1)^{(\lambda-\nu+1)/2}} \left( D_s^{\sigma, 1-\nu} \hat{L}_k^{\lambda, \sigma}, \hat{L}_n^{\lambda+\nu-1, \sigma} \right)_{\hat{w}} \\ &= \sum_{k=0}^N \frac{c_k}{(1+n)^{(\lambda+\nu-1)/2} (k+1)^{(\lambda-\nu+1)/2}} \frac{\Gamma(k+\lambda+1)}{\Gamma(k+\nu+\lambda)} \left( \hat{L}_k^{\lambda+\nu-1, \sigma}, \hat{L}_n^{\lambda+\nu-1, \sigma} \right)_{\hat{w}} \\ &= \sum_{k=0}^N \frac{c_k}{(k+1)^\lambda} \frac{\Gamma(k+\lambda+1)}{\Gamma(k+1)} \left( \frac{1}{2\sigma} \right)^{\lambda+\nu} \delta_{k,n}. \end{aligned} \quad (9)$$

Denote

$$\begin{aligned} A &= \left( \frac{1}{2\sigma} \right)^{\lambda+\nu} \begin{pmatrix} \frac{\Gamma(\lambda+1)}{\Gamma(1)1^\lambda} & & & \\ & \frac{\Gamma(\lambda+2)}{\Gamma(2)2^\lambda} & & \\ & & \ddots & \\ & & & \frac{\Gamma(\lambda+N+1)}{\Gamma(N+1)(N+1)^\lambda} \end{pmatrix} \\ F &= \left( \int_0^\infty f(x) e^{-\sigma x} L_0^{\lambda+\nu-1}(2\sigma x) dx, \dots, \frac{1}{(N+1)^{(\lambda+\nu-1)/2}} \int_0^\infty f(x) e^{-\sigma x} L_N^{\lambda+\nu-1}(2\sigma x) dx \right)^T. \end{aligned}$$

The coefficients  $C = (c_0, c_1, \dots, c_N)^T$  is obtained by solving  $AC = F$ , where the integral in  $F$  is computed by appropriate numerical quadrature.

**Remark 1** Note that our algorithm assumes  $u(0) = 0$  for (7). If  $u(0) = u_0 \neq 0$ , we can decompose the solution  $u(x) = v(x) + u_0 e^{-\sigma x}$  and solve the following associated equation for  $v(x)$ :

$$D_s^{\sigma, 1-\nu} v(x) = f(x) - \frac{u_0}{\Gamma(\nu)} \nu x^{\nu-1} e^{-\sigma x}, \quad v(0) = 0.$$

### 3.2 Substantial $(2 - \nu)$ Order FDE

Similarly, we consider equation

$$\begin{cases} D_s^{\sigma, 2-\nu} u(x) = f(x), & 0 < \nu < 1, x \in (0, \infty) \\ u(0) = 0, u'(0) = 0. \end{cases} \quad (10)$$

and take the trial space  $U_2^N = \text{span}\{(n+1)^{-\frac{\lambda-\nu+3}{2}} \hat{L}_n^{\lambda+1, \sigma}(x)\}_{n=0}^N$  and the test space  $V_2^N = V_1^N$  associated with the weight  $\hat{w}(x)$ . An appropriate Petrov–Galerkin scheme for the equation is to find  $u_N \in U_2^N$  with  $u_N(0) = u'_N(0) = 0$  such that

$$(D_s^{\sigma, 2-\nu} u_N, v)_{\hat{w}} = (f, v)_{\hat{w}}, \quad \forall v \in V_2^N.$$

Taking the form  $u_N(x) = \sum_{k=0}^N \frac{c_k}{(k+1)^{(\lambda-\nu+3)/2}} \hat{L}_k^{\lambda+1,\sigma}(x)$  and using (4) and orthogonality of the Modified Laguerre functions (3), we have

$$\begin{aligned} & \left( f, \frac{1}{(n+1)^{(\lambda+\nu-1)/2}} \hat{L}_n^{\lambda+\nu-1,\sigma} \right)_{\hat{w}} \\ &= \sum_{k=0}^N \frac{c_k}{(n+1)^{(\lambda+\nu-1)/2} (k+1)^{(\lambda-\nu+3)/2}} \left( D_s^{\sigma, 2-\nu} \hat{L}_k^{\lambda+1,\sigma}, \hat{L}_n^{\lambda+\nu-1,\sigma} \right)_{\hat{w}} \\ &= \sum_{k=0}^N \frac{c_k}{(n+1)^{(\lambda+\nu-1)/2} (k+1)^{(\lambda-\nu+3)/2}} \frac{\Gamma(\lambda+k+2)}{\Gamma(\nu+\lambda+k)} \left( \hat{L}_k^{\lambda+\nu-1,\sigma}, \hat{L}_n^{\lambda+\nu-1,\sigma} \right)_{\hat{w}} \\ &= \sum_{k=0}^N \frac{c_k}{(k+1)^{\lambda+1}} \frac{\Gamma(\lambda+k+2)}{\Gamma(k+1)} \left( \frac{1}{2\sigma} \right)^{\lambda+\nu} \delta_{k,n}. \end{aligned}$$

Finally, we solve a diagonal system  $AC = F$ , where

$$\begin{aligned} A &= \left( \frac{1}{2\sigma} \right)^{\lambda+\nu} \begin{pmatrix} \frac{\Gamma(\lambda+2)}{\Gamma(1)1^{\lambda+1}} & & & \\ & \frac{\Gamma(\lambda+3)}{\Gamma(2)2^{\lambda+1}} & & \\ & & \ddots & \\ & & & \frac{\Gamma(\lambda+N+2)}{\Gamma(N+1)(N+1)^{\lambda+1}} \end{pmatrix} \\ F &= \left( \int_0^\infty f(x) e^{-\sigma x} L_0^{\lambda+\nu-1}(2\sigma x) dx, \dots, \frac{1}{(N+1)^{(\lambda+\nu-1)/2}} \int_0^\infty f(x) e^{-\sigma x} L_N^{\lambda+\nu-1}(2\sigma x) dx \right)^T. \end{aligned}$$

**Remark 2** The scaling factors in the test space and the trial space play the role of precondition factor for the matrix  $A$ .

**Remark 3** We adopt traditional approach to impose initial condition for (7) and (10). Moreover, for (10) with non-homogeneous initial conditions, we can take a similar process as that in Remark 1 to make a transformation.

### 3.3 Convergence Analysis

In this section, a rigorous error analysis for our PG schemes is carried out. A careful transform of the schemes reveals that they are equivalent to standard weighted  $L^2$  projection for an invariant of the source term  $f(x)$ .

**Theorem 1** Let  $u$  be the solution of (7) and  $u_N$  be its Petrov–Galerkin approximation (8). If  $g_f(x) := f(x)e^{\sigma x}x^{1-\lambda-\nu} \in B_{w^{\lambda+\nu-1}}^m([0, \infty))$ , where  $0 < \lambda, \nu < 1$  and  $\sigma > 0$ , then

$$\|D_s^{\sigma, 1-\nu}(u - u_N)\|_{\hat{w}} \leq CN^{-m/2} \|\partial_x^m g_f\|_{w^{\lambda+\nu+m-1}}.$$

*Proof* From (9), we have for any  $v \in V_1^N$ ,

$$(f - D_s^{\sigma, 1-\nu}u_N, v)_{\hat{w}} = 0.$$



Hence, our problem is equivalent to finding the  $L^2_{\hat{w}}$  projection of  $f$  in

$$\text{span}\{D_s^{\sigma, 1-\nu} \hat{L}_k^{\lambda, \sigma}\} = \text{span}\left\{\frac{\Gamma(\lambda + k + 1)}{\Gamma(\nu + \lambda + k)} \hat{L}_k^{\lambda + \nu - 1, \sigma}, 0 \leq k \leq N\right\}$$

by testing on  $V_1^N$ .

Next, we define the operator

$$(\hat{\pi}_N f)(x) := x^{\lambda + \nu - 1} e^{-\sigma x} (\pi_N g_f)(x),$$

where  $\pi_N$  is the  $L^2$  projection with respect to  $w^{\lambda + \nu - 1}(x)$ . Therefore,

$$0 = (\hat{\pi}_N f - f, \psi)_{\hat{w}} = (\pi_N g_f - g_f, v_N)_{w^{\lambda + \nu - 1}}, \quad \forall v_N \in P_N. \quad (11)$$

This means our method boils down to finding the standard  $L^2$  projection for the function  $f(x)e^{\sigma x}x^{1-\lambda-\nu}$  with respect to the weight  $w^{\lambda + \nu - 1}(x)$ .

Therefore, by Lemma 2,

$$\|D_s^{1-\nu}(u - u_N)\|_{\hat{w}}^2 = \|f - \hat{\pi}_N f\|_{\hat{w}}^2 = \|\pi_N g_f - g_f\|_{w^{\lambda + \nu - 1}}^2 \leq CN^{-m} \|\partial_x^m g\|_{w^{\lambda + \nu + m - 1}}^2.$$

□

Similarly, for substantial  $(2 - \nu)$  order problem, we have

**Theorem 2** Let  $u$  be the solution of (10) and  $u_N$  be its corresponding Petrov–Galerkin approximation. If  $g_f(x) := f(x)e^{\sigma x}x^{1-\lambda-\nu} \in B_{w^{\lambda + \nu - 1}}^m([0, \infty))$ , where  $0 < \lambda, \nu < 1$  and  $\sigma > 0$ , then

$$\|D_s^{\sigma, 2-\nu}(u - u_N)\|_{\hat{w}} \leq CN^{-m/2} \|\partial_x^m g_f\|_{w^{\lambda + \nu + m - 1}}.$$

*Proof* Omitted. □

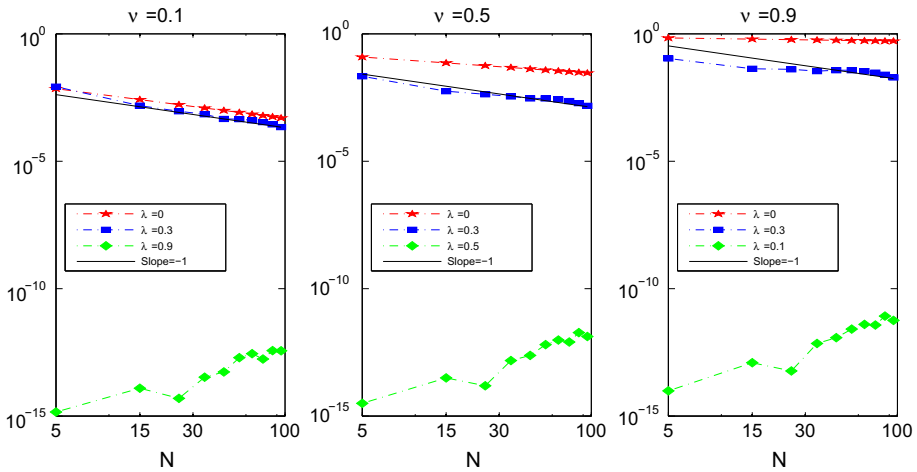
**Remark 4** If  $\lambda = 1 - \nu$  is chosen in our theorems, then the standard  $L^2$  estimate of  $D_s^{\sigma, 1-\nu} u_N$  ( $D_s^{\sigma, 2-\nu} u_N$ ) to  $D_s^{\sigma, 1-\nu} u$  ( $D_s^{\sigma, 2-\nu} u$ ) is obtained.

**Remark 5** It is apparent that the optimality of Lemma 2 leads to the optimality of our theorems. The convergence rate of the PG method depends on the regularity of  $g_f$  instead of  $f$  itself. Therefore, we are allowed to adjust the parameter  $\lambda$  according to the given data  $f$  to maximize the smoothness of  $g$ . Moreover, [25, Theorem 9.1.5] implies that  $g_f \in B_{w^{\lambda + \nu - 1}}^m([0, \infty))$  leads to equiconvergence of  $\pi_N g_f$  and Fourier series to  $g_f$ , and thus the equiconvergence of corresponding series to  $f$ .

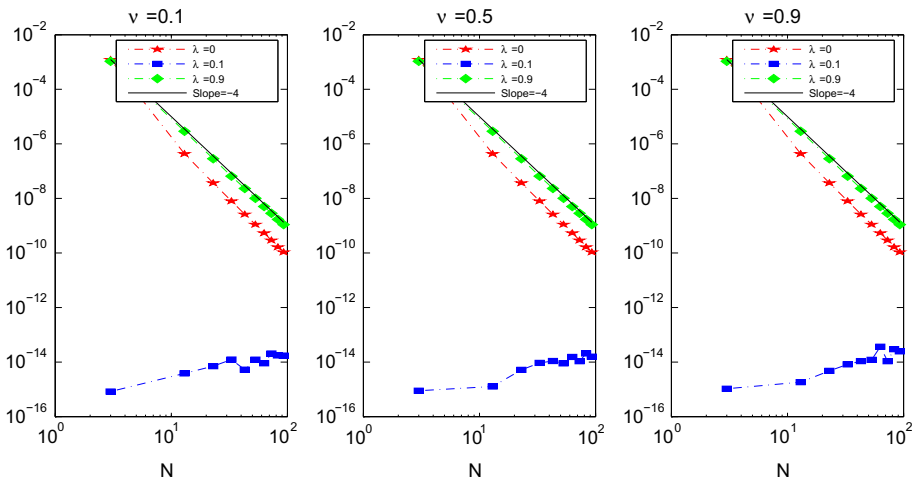
### 3.4 Numerical Experiments

In this subsection, numerical errors are measured in  $\|\cdot\|_{\infty}$  and computed by sampling at the points  $x = 0, 0.01, \dots, 9.99, 10$ . The right hand side  $F$  of our algorithm is approximated by  $2N$ -point Gauss-Laguerre numerical quadrature for each different  $N$ .

**Example 1** We first consider the Eq. (7) with  $\sigma = 2$  and  $f(x) = e^{-\sigma x}$ . Through the error estimate in Theorem 1,  $\lambda = 1 - \nu$  leads to an entire function  $g_f(x)$ , which further indicates an enhanced convergence rate. Indeed, for this case, the true solution sets root in our approximation space  $U_1$  after a small  $N$ , and therefore only round-off errors are left. However, for other choice of  $\lambda$ 's, algebraic convergence rate is observed as the theorem predicts, see Fig. 1. We also observe a convergence rate of  $\mathcal{O}(N^{-1})$ , which is better than our theoretical



**Fig. 1** (Example 1):  $L^\infty$  error of the approximation to the true solution of  $D_s^{\sigma, 1-\nu} u(x) = f(x)$ ,  $x \in [0, \infty)$ ,  $u(0) = 0$ , for spectral Petrov–Galerkin method



**Fig. 2** (Example 2):  $L^\infty$  error of the approximation to the true solution of  $D_s^{\sigma, 2-\nu} u(x) = f(x)$ ,  $x \in [0, \infty)$ ,  $u(0) = 0$ ,  $u'(0) = 0$  for spectral Petrov–Galerkin method

prediction  $\mathcal{O}(N^{-0.5})$  since  $g_f(x) \in B_{w^{\lambda+\nu-1}}^1([0, \infty))$  if  $\lambda + \nu < 1$ . Note that the error in our numerical experiment is measured in  $L^\infty$  norm, whereas in our theoretical prediction, it is measured in the weighted  $L^2$  norm of the fractional derivative.

**Example 2** Next, we consider Eq. (10) with true solution  $f(x) = B(5.1, \nu)(\nu + 4.1)(\nu + 3.1)x^{\nu+2.1}e^{-\sigma x} / \Gamma(\nu)$  and  $\sigma = 2$ . Theorem 2 indicates that the convergence rate depends on the regularity of  $g(x) = f(x)e^{\sigma x}x^{1-\lambda-\nu} \in B_{w^{\lambda+\nu-1}}^6([0, \infty))$  for all  $0 < \lambda, \nu < 1$ . As expected, we only observe round-off errors for  $\lambda = 0.1$  after a small  $N$ . For other choice of  $\lambda$ 's, we observe algebraic convergence rate  $\mathcal{O}(N^{-4})$ , which is also better than our theoretical prediction  $\mathcal{O}(N^{-3})$ , see Fig. 2 for details.

## 4 Spectral Collocation Method

As has been shown, our spectral Petrov–Galerkin method yields diagonal linear systems by carefully choosing trial space and test space regarding (7) and (10). However, PG schemes in general have difficulties in the treatment of nonlinear FPDEs, since no straightforward variational form can be efficiently obtained for such problems [31]. In this section, we shall exploit substantial collocation methods, which are relatively easy to implement and can overcome the aforementioned challenges [31].

### 4.1 Substantial (1 – $\nu$ ) Order FDE

Let  $\{x_j, w_j\}_{j=0}^N$  is the Laguerre–Gauss–Radau (LGR) points and weights with respect to the weight  $x^\lambda e^{-2\sigma x}$ . As the PG method, we seek an approximation of  $u$

$$u_N \in \text{span} \{ \hat{L}_n^{\lambda, \sigma}(x), 0 \leq n \leq N-1, x \in [0, \infty) \}.$$

For the sake of derivation of collocation matrix, we rewrite  $u_N$  in nodal expansion, i.e.

$$u_N(x) = \sum_{j=0}^N u_N(x_j) h_j(x),$$

where  $h_j(x)$  is our interpolant function on the points  $\{x_j\}_{j=1}^N$ ,

$$h_j(x) = \frac{x^\lambda e^{-\sigma x}}{x_j^\lambda e^{-\sigma x_j}} \prod_{i=1, i \neq j}^N \frac{(x - x_i)}{(x_j - x_i)} := \frac{x^\lambda e^{-\sigma x}}{x_j^\lambda e^{-\sigma x_j}} l_j(x), \quad 1 \leq j \leq N.$$

Thereby, from (6) and the initial condition

$$\begin{aligned} D_s^{\sigma, 1-\nu} u_N(x) &= \sum_{j=1}^N u(x_j) D_s^{\sigma, 1-\nu} h_j(x) \\ &= \sum_{j=1}^N u(x_j) \frac{1}{x_j^\lambda e^{-\sigma x_j}} \sum_{k=0}^{N-1} \beta_k^j [D_s^{1-\nu} \hat{L}_k^\lambda(x)] \\ &= \sum_{j=1}^N u(x_j) \frac{1}{x_j^\lambda e^{-\sigma x_j}} \sum_{k=0}^{N-1} \beta_k^j \frac{\Gamma(\lambda + k + 1)}{\Gamma(\nu + \lambda + k)} \hat{L}_k^{\lambda+\nu-1}(x). \end{aligned}$$

Next, let us find an explicit expression for  $\beta_k^j$  such that  $l_j(x) = \sum_{k=0}^{N-1} \beta_k^j L_k^\lambda(2\sigma x)$ . Since 0 is excluded in the collocation points set,

$$\begin{aligned} \beta_k^j &= \frac{1}{\|L_k^\lambda(2\sigma x)\|_{w^\lambda}^2} \int_0^\infty l_j(x) L_k^\lambda(x) x^\lambda e^{-2\sigma x} dx, \\ &= \frac{(2\sigma)^{1+\lambda} k!}{\Gamma(k + \lambda + 1)} \left[ w_0 l_j(0) \frac{\Gamma(k + \lambda + 1)}{k! \Gamma(\lambda + 1)} + w_j L_k^\lambda(2\sigma x_j) \right]. \end{aligned} \quad (12)$$

From the orthogonality of Laguerre polynomials and the fact that the Laguerre–Gauss–Radau is exact for all polynomial of order up to  $2N$ , one easily has

$$\begin{aligned} 0 &= \int_0^\infty l_j(x) L_N^\lambda(2\sigma x) x^\lambda e^{-2\sigma x} dx, \\ &= w_0 l_j(0) \frac{\Gamma(N + \lambda + 1)}{N! \Gamma(\lambda + 1)} + w_j L_N^\lambda(2\sigma x_j). \end{aligned} \quad (13)$$

Solving for  $l_j(0)$  from (13) and substituting it into (12), we obtain

$$\beta_k^j = (2\sigma)^{\lambda+1} w_j \left[ \frac{k! L_k^\lambda(2\sigma x_j)}{\Gamma(k + \lambda + 1)} - \frac{N! L_N^\lambda(2\sigma x_j)}{\Gamma(N + \lambda + 1)} \right]. \quad (14)$$

Consequently, we evaluate the  $D_s^{1-\nu} u_N(x)$  at collocation points and obtain

$$\begin{aligned} D_s^{\sigma, 1-\nu} u_N(x) \Big|_{x=x_i} &= \sum_{j=1}^N u(x_j) \frac{1}{x_j^\lambda e^{-\sigma x_j}} \sum_{k=0}^{N-1} \beta_k^j \frac{\Gamma(\lambda + k + 1)}{\Gamma(\nu + \lambda + k)} \hat{L}_k^{\lambda+\nu-1}(x_i) \\ &= \sum_{j=1}^N \mathbf{D}_{ij} u(x_j), \end{aligned}$$

where  $\mathbf{D}_{ij}$  are the entries of the  $N \times N$  collocation matrix  $\mathbf{D}$  and

$$\mathbf{D}_{ij} = \frac{(2\sigma)^{\lambda+1} w_j}{x_j^\lambda e^{-\sigma x_j}} \sum_{k=0}^{N-1} \left[ \frac{k! L_k^\lambda(2\sigma x_j)}{\Gamma(k + \lambda + 1)} - \frac{N! L_N^\lambda(2\sigma x_j)}{\Gamma(N + \lambda + 1)} \right] \frac{\Gamma(\lambda + k + 1)}{\Gamma(\nu + \lambda + k)} \hat{L}_k^{\lambda+\nu-1}(x_i), \quad (15)$$

where  $1 \leq i, j \leq N$ .

## 4.2 Substantial $(2 - \nu)$ Order FDE

In this subsection, we consider the spectral collocation method for (10). Let  $\{x_j, w_j\}_{j=0}^N$  be the Laguerre–Gauss–Radau points and weights with respect to the weight  $x^{\lambda+1} e^{-2\sigma x}$ . Following the spirit of PG method, we seek an approximation

$$u_N \in \text{span} \{ \hat{L}_n^{\lambda+1}(x), 0 \leq n \leq N-1 \}, x \in [0, \infty)$$

such that it satisfies the initial conditions. As before, we rewrite it in nodal expansion form

$$u_N(x) = \sum_{j=0}^N u(x_j) h_j(x),$$

where  $h_{j(x)}$  is of the form

$$h_j(x) = \frac{x^{\lambda+1} e^{-\sigma x}}{x_j^{\lambda+1} e^{-\sigma x_j}} \prod_{i=1, i \neq j}^N \left( \frac{x - x_i}{x_j - x_i} \right) := \frac{x^{\lambda+1} e^{-\sigma x}}{x_j^{\lambda+1} e^{-\sigma x_j}} l_j(x), 1 \leq j \leq N.$$

By a similar process in (12)–(14), we obtain an explicit expression for  $\beta_k^j$  such that  $l_j(x) = \sum_{k=0}^{N-1} \beta_k^j L_k^{\lambda+1}(2\sigma x)$ .

$$\beta_k^j = (2\sigma)^{\lambda+2} w_j \left[ \frac{k! L_k^{\lambda+1}(2\sigma x_j)}{\Gamma(k + \lambda + 2)} - \frac{N! L_N^{\lambda+1}(2\sigma x_j)}{\Gamma(N + \lambda + 2)} \right]. \quad (16)$$

We then obtain the collocation matrix

$$\mathbf{D}_{ij} = \frac{w_j (2\sigma)^{\lambda+2}}{x_j^{\lambda+1} e^{-\sigma x_j}} \sum_{k=0}^{N-1} \left[ \frac{k! L_k^{\lambda+1}(2\sigma x_j)}{\Gamma(k + \lambda + 2)} - \frac{N! L_N^{\lambda+1}(2\sigma x_j)}{\Gamma(N + \lambda + 2)} \right] \frac{\Gamma(\lambda + k + 2)}{\Gamma(\nu + \lambda + k)} \hat{L}_k^{\lambda+\nu-1}(x_i) \quad (17)$$

where  $1 \leq i, j \leq N$ .

**Remark 6** The computational cost for computing the matrix  $\mathbf{D}$  from (15) or (17) may be high since it is a full matrix in general. However, this task can be done once for all. The strength is remarkable if one solves a system of fractional differential equations repeatedly.

### 4.3 Convergence Analysis

We start with an estimate of interpolation error on Laguerre–Gauss–Radau points.

**Lemma 3** [10, Theorem 3.7] *Let  $\alpha > -1$ . If  $u \in B_{w^{\alpha-1}}^m([0, \infty)) \cap B_{w^\alpha}^m([0, \infty))$  with  $1 \leq m \leq N + 1$ , then*

$$\|I_N^\alpha u - u\|_{w^\alpha} \leq C N^{(1-m)/2} (\|\partial_x^m u\|_{w^{\alpha-1+m}} + (\ln N)^{1/2} \|\partial_x^m u\|_{w^{\alpha+m}}),$$

where  $I_N^\alpha$  is the interpolation operator on  $(N+1)$  Laguerre–Gauss–Radau points with respect to  $x^\alpha e^{-2\sigma x}$ .

**Theorem 3** *Let  $u$  and  $u_N$  be the solution of (7) and its spectral collocation method with the collocation matrix given by (15), respectively. Let  $g_f(x) = f(x)e^{\sigma x}x^{1-\lambda-\nu} \in B_{w^{\lambda+\nu-1}}^m([0, \infty)) \cap B_{w^{\lambda+\nu}}^m([0, \infty))$ , where  $0 < \lambda, \nu < 1$  and  $\sigma > 0$ . Then*

$$\|D_s^{\sigma, 1-\nu}(u - u_N)\|_{\hat{w}} \leq C N^{(1-m)/2} (\|\partial_x^m g_f\|_{w^{\lambda+\nu+m-1}} + (\ln N)^{1/2} \|\partial_x^m g_f\|_{w^{\lambda+\nu+m}}).$$

*Proof* Let  $\{x_i, w_i\}_{i=0}^N$  be the  $(N+1)$  Laguerre–Gauss–Radau quadrature points and weights associated with the weight  $x^\lambda e^{-2\sigma x}$ . Our collocation scheme reads as

$$D_s^{\sigma, 1-\nu} u_N(x_i) = f(x_i), \quad i = 0, \dots, N.$$

Multiplying both sides of the above equation by  $(n+1)^{1-\nu} x_i^{-\lambda} e^{\sigma x_i} L_n^{\lambda+\nu-1}(x_i) w_i$  and summing up, we obtain

$$\begin{aligned} (n+1)^{1-\nu} \sum_{i=0}^N D_s^{\sigma, 1-\nu} u_N(x_i) x_i^{-\lambda} e^{\sigma x_i} L_n^{\lambda+\nu-1}(2\sigma x_i) w_i \\ = (n+1)^{1-\nu} \sum_{i=0}^N f(x_i) x_i^{-\lambda} e^{\sigma x_i} L_n^{\lambda+\nu-1}(2\sigma x_i) w_i, \end{aligned}$$

which is equivalent to

$$\begin{aligned} (D_s^{\sigma, 1-\nu} u_N, (n+1)^{1-\nu} \hat{L}_n^{\lambda+\nu-1})_{\hat{w}} &= (g_f, (n+1)^{1-\nu} L_n^{\lambda+\nu-1}(2\sigma x))_{w^{\lambda+\nu-1}}^* \\ &= (I_N g_f, (n+1)^{1-\nu} L_n^{\lambda+\nu-1}(2\sigma x))_{w^{\lambda+\nu-1}} \end{aligned}$$

by the exactness of the  $(N + 1)$ -point Laguerre–Gauss–Radau quadrature. Here,  $*$  indicates numerical quadrature. Next, we consider an auxiliary equation

$$\begin{aligned}(D_s^{\sigma, 1-\nu} \bar{u}_N, (n+1)^{1-\nu} \hat{L}_n^{\lambda+\nu-1, \sigma})_{\hat{w}} &= (g_f, (n+1)^{1-\nu} L_n^{\lambda+\nu-1}(2\sigma x))_{w^{\lambda+\nu-1}} \\ &= (f, (n+1)^{1-\nu} \hat{L}_n^{\lambda+\nu-1, \sigma})_{\hat{w}}.\end{aligned}$$

Denote  $(D_s^{\sigma, 1-\nu} \bar{u}_N)(x) := (\hat{\pi}_N f)(x) = x^{\lambda+\nu-1} e^{-\sigma x} (\pi_N g_f)(x)$ . The problem is simplified to

$$(f - \hat{\pi}_N f, (n+1)^{1-\nu} \hat{L}_n^{\lambda+\nu-1, \sigma})_{\hat{w}} = 0, \quad 0 \leq n \leq N,$$

which is clearly a Galerkin problem as (11).

By Lemma 2, assuming  $g_f \in B_{w^{\lambda+\nu-1}}^m([0, \infty))$ ,

$$\|D_s^{\sigma, 1-\nu} u - D_s^{\sigma, 1-\nu} \bar{u}_N\|_{\hat{w}} = \|f - \hat{\pi}_N f\|_{\hat{w}^{1-\lambda-\nu}} \leq C N^{-m/2} \|\partial_x^m g_f\|_{w^{\lambda+\nu+m-1}}. \quad (18)$$

Now, let us consider the effect of numerical integration. Lemma 3 directly implies

$$\begin{aligned}& \sup_{L_n^{\lambda+\nu-1} \in P_{N-1}} \frac{|(f, \hat{L}_n^{\lambda+\nu-1, \sigma})_{\hat{w}^{1-\lambda-\nu}} - (I_N g_f, L_n^{\lambda+\nu-1}(2\sigma x))_{w^{\lambda+\nu-1}}|}{\|L_n^{\lambda+\nu-1}\|_{w^{\lambda+\nu-1}}} \\ &= \sup_{L_n^{\lambda+\nu-1} \in P_{N-1}} \frac{|(g_f - I_N g_f, L_n^{\lambda+\nu-1}(2\sigma x))_{w^{\lambda+\nu-1}}|}{\|L_n^{\lambda+\nu-1}\|_{w^{\lambda+\nu-1}}} \\ &\leq C N^{(1-m)/2} (\|\partial_x^m g_f\|_{w^{\lambda+\nu+m-1}} + (\ln N)^{1/2} \|\partial_x^m g_f\|_{w^{\lambda+\nu+m-1}}),\end{aligned} \quad (19)$$

Combining (18) and (19), the result is then followed by an application of the Strang's lemma.  $\square$

**Theorem 4** *Let  $u$  and  $u_N$  be the solution of (10) and our collocation method with collocation matrix given by (17). Let  $g_f(x) = f(x)e^{\sigma x}x^{1-\lambda-\nu} \in B_{w^{\lambda+\nu-1}}^m([0, \infty)) \cap B_{w^{\lambda+\nu}}^m([0, \infty))$ , where  $0 < \lambda, \nu < 1$  and  $\sigma > 0$ . Then*

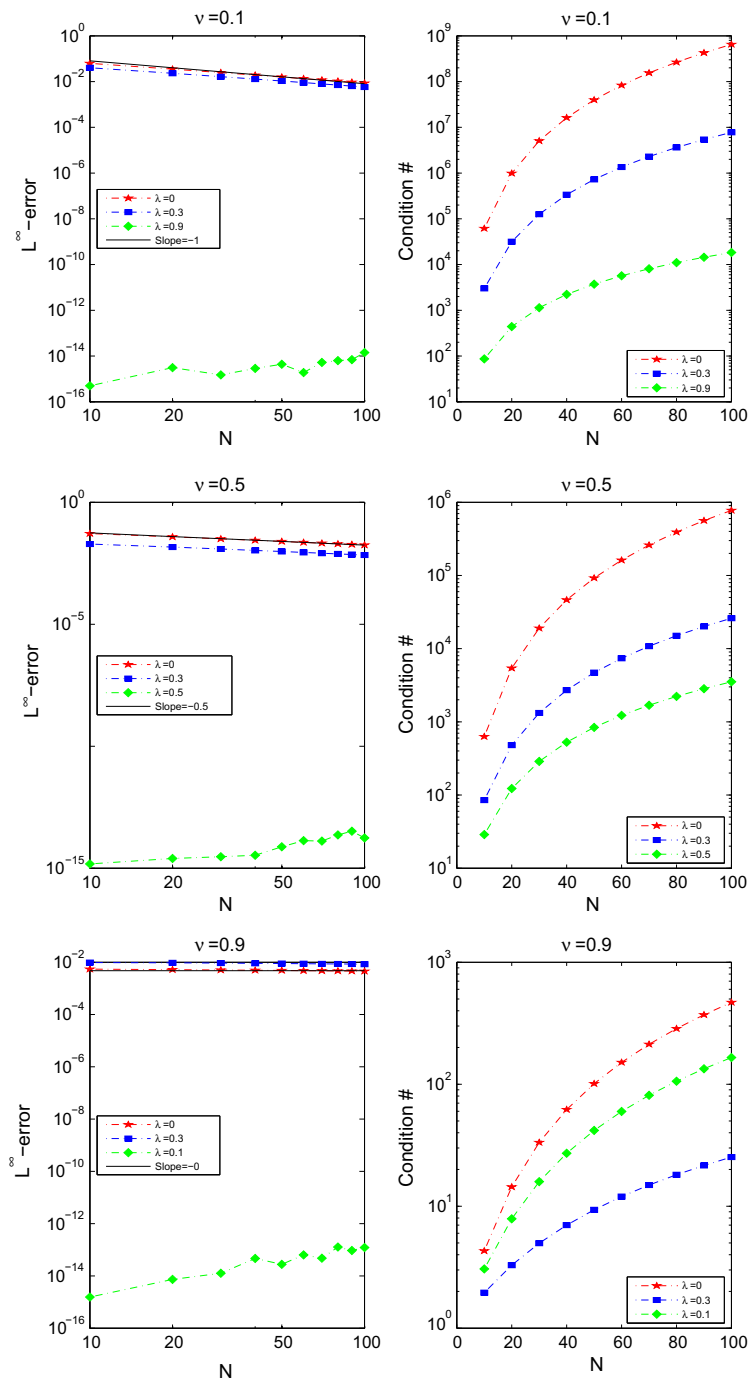
$$\|D_s^{\sigma, 2-\nu}(u - u_N)\|_{\hat{w}} \leq C N^{(1-m)/2} (\|\partial_x^m g_f\|_{w^{\lambda+\nu+m-1}} + (\ln N)^{1/2} \|\partial_x^m g_f\|_{w^{\lambda+\nu+m}}).$$

*Proof* The proof is the same as that of Theorem 3 and thus is omitted.  $\square$

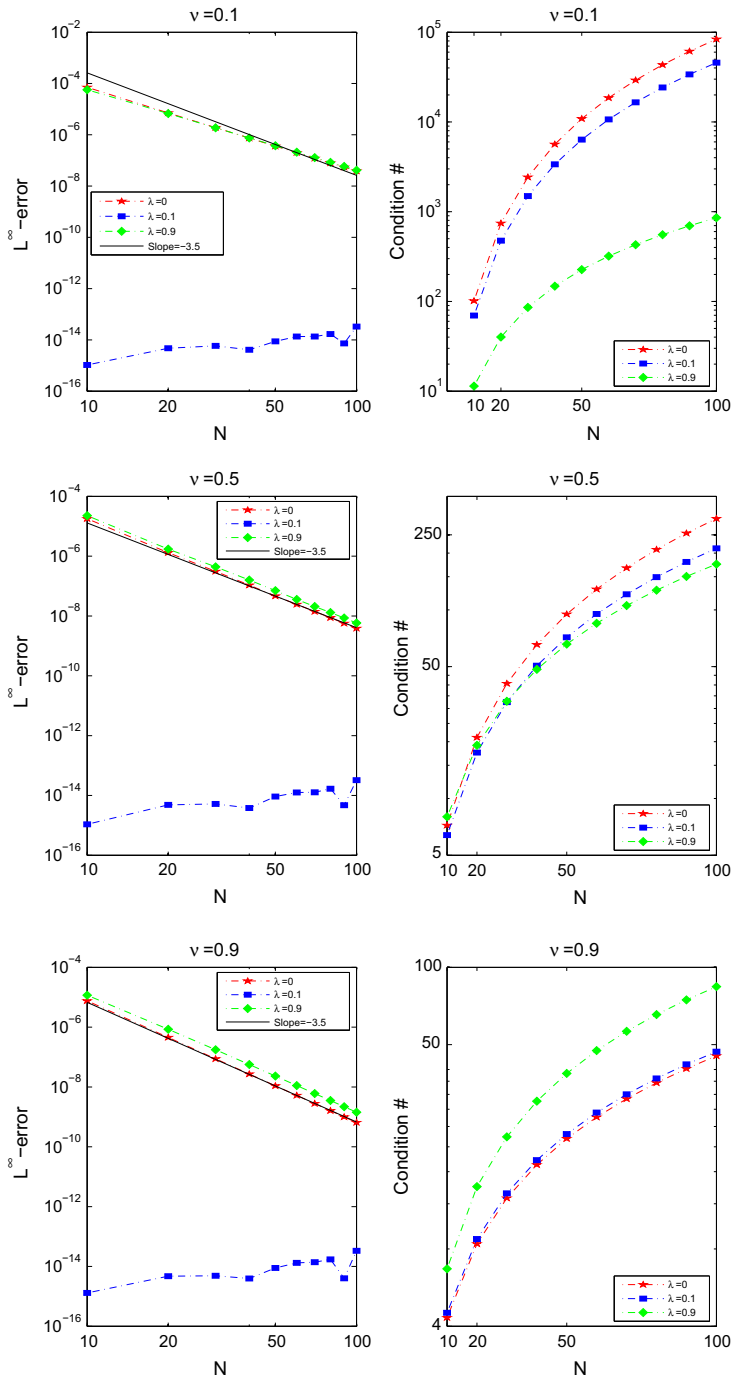
## 4.4 Numerical Experiments

**Example 3** We consider (7) to test the efficiency of our collocation method. The collocation matrix **D** is obtained based upon (15) by collocating on the LGR points associated with the weight  $x^\lambda e^{-2\sigma x}$  and the  $L^\infty$  error is obtained by sampling at these points also. In this example, we choose  $\sigma = 2$  and  $f(x) = e^{-\sigma x}$ . Numerical behaviors for different number of collocation points are presented in Fig. 3. We observe that the numerical errors of the collocation method for different  $\lambda$ 's follow a similar pattern as the PG method. In particular, when  $\lambda = 1 - \nu$ ,  $g_f(x) = 1 \in B_{w_0}^m([0, \infty))$  for arbitrarily large  $m$ . We only observe round-off errors for this case. However, the condition number of the collocation matrix grows very quickly as the number of collocation points  $N$  grows for all  $\lambda$ 's.

**Example 4** For (10), we choose  $f(x) = B(5.1, \nu)(\nu + 4.1)(\nu + 3.1)x^{\nu+2.1}e^{-\sigma x} / \Gamma(\nu)$  and  $\sigma = 2$  and collocate the equation on LGR points with respect to the weight  $x^{\lambda+1}e^{-2\sigma x}$  and  $\sigma = 2$ . Again, the  $L^\infty$  error is obtained by sampling at our collocation points. In Fig. 4, we only observe round-off errors for  $\lambda = 0.1$  and algebraic convergence rate  $\mathcal{O}(N^{-3.5})$  for other  $\lambda$ 's, which is in contrast with  $\mathcal{O}(N^{-2.5})$  predicted by Theorem 4.



**Fig. 3** (Example 3):  $L^\infty$  error of the approximation to the true solution of  $D_s^{1-\nu}u(x) = f(x)$ ,  $x \in [0, \infty)$ ,  $u(0) = 0$  for Laguerre–Gauss–Radau points. The *right column* is plots of condition numbers of direct collocation differential matrix



**Fig. 4** (Example 4):  $L^\infty$  error of the approximation to the true solution of  $D_s^{\sigma, 2-\nu} u(x) = f(x)$ ,  $x \in [0, \infty)$ ,  $u(0) = 0$ ,  $u'(x) = 0$  for Laguerre–Gauss–Radau points. The right column is plots of condition numbers of direct collocation differential matrix



## 5 Superconvergence of Petrov–Galerkin Method

Let  $u(x)$  and  $u_N(x)$  be the true solution and PG approximation of (7) and (10). In this section, our goal is to identify

- superconvergence points of the PG method for substantial fractional derivative. In other words, we specify certain set of points  $y_j$  such that  $D_s^{\sigma, m-\nu} u_N$  superconverges to  $D_s^{\sigma, m-\nu} u$  in the sense that

$$N^\alpha |D_s^{m-\nu}(u - u_N)(y_j)| \leq C \max_{x \in [0, \infty)} |D_s^{m-\nu}(u - u_N)(x)|, \quad \alpha > 0, \quad m = 1 \text{ or } 2;$$

- superconvergence points of the PG approximation for function value, namely, find certain set points  $z_j$  such that  $u_N$  superconverges to  $u$  in the sense that

$$N^\beta |(u - u_N)(z_j)| \leq C \max_{x \in [0, \infty)} |(u - u_N)(x)|, \quad \beta > 0, \quad m = 1 \text{ or } 2,$$

where  $C$  is a constant independent of  $N$ .

### 5.1 Superconvergence Points

**Theorem 5** Assume  $g_f = f(x)e^{\sigma x}x^{1-\lambda-\nu} \in B_{w^{\lambda+\nu-1}}^m([0, \infty))$ , where  $0 < \lambda, \nu < 1$  and  $\sigma > 0$ . The substantial fractional derivative  $D_s^{1-\nu} u_N$  of our spectral Petrov–Galerkin method for (7) superconverges to  $D_s^{1-\nu} u$  at zeros of  $L_{N+1}^{\lambda+\nu-1}(2\sigma x)$  and  $u_N$  itself superconverges to  $u$  at zeros of  $L_{N+1}^{\lambda}(2\sigma x)$ .

*Proof* Since  $B_{w^{\lambda+\nu-1}}^m([0, \infty)) \subset L_{w^{\lambda+\nu-1}}^2([0, \infty))$  and  $\{L_n^{\lambda+\nu-1}(y)\}_{n=0}^\infty$  is complete in the weighted space  $L_{w^{\lambda+\nu-1}}^2([0, \infty))$ , we clearly have

$$g_f(x) = \sum_{k=0}^{\infty} c_k L_k^{\lambda+\nu-1}(2\sigma x)$$

for some  $\{c_k\}_{k=0}^\infty$ , which indicates

$$f(x) = x^{\lambda+\nu-1} e^{-\sigma x} \sum_{k=0}^{\infty} c_k L_k^{\lambda+\nu-1}(2\sigma x). \quad (20)$$

Recall that operators  $\hat{\pi}_N$  and  $\pi_N$  satisfy

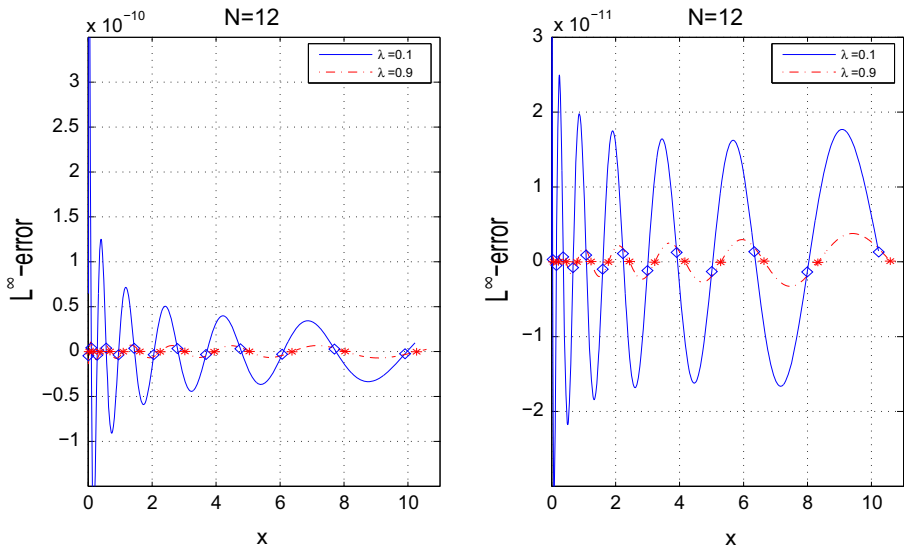
$$0 = (\hat{\pi}_N f - f, \psi)_{\hat{w}} = (\pi_N g_f - g_f, v_N)_{w^{\lambda+\nu-1}}, \quad \forall v_N \in P_N.$$

Hence,  $\pi_N$  is exactly a truncation operator up to the first  $N + 1$  terms by the orthogonality (3) and

$$\pi_N g_f = \sum_{k=0}^N c_k L_k^{\lambda+\nu-1}(2\sigma x),$$

which further implies

$$\hat{\pi}_N f = \sum_{k=0}^N c_k \hat{L}_k^{\lambda+\nu-1, \sigma}(x).$$



**Fig. 5** (Example 5): (Left)  $L^\infty$  error of the approximation of the fractional derivative with different  $\lambda$ 's and their superconvergence points, i.e. zeros of  $L_{N+1}^{\lambda+\nu-1}(2\sigma x)$ ; (Right)  $L^\infty$  error of the approximation of the function value with different  $\lambda$ 's and their superconvergence points, i.e. zeros of  $L_{N+1}^\lambda(2\sigma x)$  to  $D_s^{\sigma, 1-\nu} u(x) = f(x)$ ,  $x \in [0, \infty)$ ,  $u(0) = 0$

Therefore, our Petrov–Galerkin method exactly yields the first  $N + 1$  terms in (20) as an approximation and leaves others as a remainder, in which, the major term is clearly  $c_{N+1} L_{N+1}^{\lambda+\nu-1}(2\sigma x)$ . Thus, at zeros of  $L_{N+1}^{\lambda+\nu-1}(2\sigma x)$ , this major term vanishes and the fractional derivative of our approximation superconverges to that of the true solution.

From (20) and (6), we easily deduce that under the assumption,

$$u(x) = \sum_{k=0}^{\infty} c_k \hat{L}_k^{\lambda, \sigma}(x) \quad (21)$$

and thus the superconvergence points of  $u_N = \sum_{k=0}^N c_k \hat{L}_k^{\lambda, \sigma}(x)$  to  $u$  are the zeros of  $L_{N+1}^\lambda(2\sigma x)$ .  $\square$

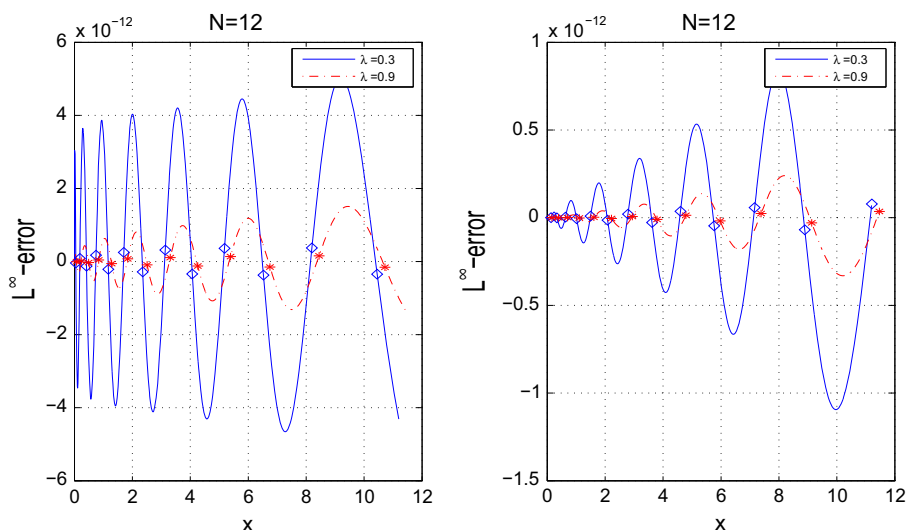
Similarly, for Eq. (10), we have

**Theorem 6** Assume  $g_f = f(x)e^{\sigma x}x^{1-\lambda-\nu} \in B_{w^{\lambda+\nu-1}}^m([0, \infty))$ , where  $0 < \lambda, \nu < 1$  and  $\sigma > 0$ . The substantial fractional derivative  $D_s^{2-\nu} u_N$  of our spectral Petrov–Galerkin method for (10) superconverges to  $D_s^{2-\nu} u$  at zeros of  $L_{N+1}^{\lambda+\nu-1}(2\sigma x)$  and  $u_N$  superconverges to  $u$  at zeros of  $L_{N+1}^{\lambda+1}(2\sigma x)$ .

*Proof* Omitted.  $\square$

## 5.2 Numerical Experiments

**Example 5** We choose  $\nu = 0.3$ ,  $u(x) = x^{14.3}e^{-\sigma x}/10^{14}$  and its corresponding  $f(x)$  in (7). The scaling factor  $1/10^{14}$  is chosen such that the modulus of coefficients  $(c_k)_{k=0}^N$  in our



**Fig. 6** (Example 6): (Left):  $L^\infty$  error of fractional derivative with different  $\lambda$ 's and their superconvergence points, i.e. zeros of  $L_{N+1}^{\lambda+\nu-1}(2\sigma x)$ ; (Right):  $L^\infty$  error of function value with different  $\lambda$ 's and their superconvergence points, i.e. zeros of  $L_{N+1}^{\lambda+1}(2\sigma x)$  to  $D_s^{\sigma, 2-\nu}u(x) = f(x)$ ,  $x \in [0, \infty)$ ,  $u(0) = u'(0) = 0$

algorithm are mild.  $L^\infty$  errors for both fractional derivative and function value approximation for different  $\lambda$  are presented. For clarity, superconvergence points predicted by our theorems are also plotted.

**Example 6** Consider the model problem (10) with  $\nu = 0.3$ ,  $u(x) = x^{14.1}e^{-\sigma x}/10^{12}$ . As in the example 5,  $1/10^{12}$  is also a scaling factor. We plot the  $L^\infty$  error of both fractional derivative and function value for different  $\lambda$ 's. Superconvergence points from our theoretical prediction are plotted for a comparison.

In Figs. 5 and 6,  $L^\infty$  error of both fractional derivative and function value of the true solution with  $N = 12$  are plotted. For different choice of  $\lambda = 0.1$  and  $0.9$ , errors on associated superconvergence points are marked. Clearly, errors at these points are much smaller than the global maximum error.

## 6 Conclusion

We have considered Petrov–Galerkin methods and spectral collocation methods for two types of substantial fractional differential equations. Four different algorithms for the model problems have been proposed, analyzed and tested. In particular, well-conditioned Petrov–Galerkin methods for (7) and (10) have been constructed, which yield diagonal linear systems. Error estimates have been derived with convergences rate depending only on the smoothness of the given data. Moreover, superconvergence points of our PG method are identified. In addition, a spectral collocation method for these two types of equations are also developed. Explicit collocation matrices are developed and associated error estimates are carried out. It is noteworthy that our analysis is tailored to the model problems (7) and (10). Substantial

fractional differential equations with a lower order term require a different treatment and a further investigation, which will be the subject of our future work.

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