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ORIGINAL PAPER

A New Spectral Method Using Nonstandard Singular Basis Functions for Time-Fractional Differential Equations

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Abstract
In this paper, we introduce new non-polynomial basis functions for spectral approximation of time-fractional partial differential equations (PDEs). Different from many other approaches, the nonstandard singular basis functions are defined from some generalised Birkhoff interpolation problems through explicit inversion of some prototypical fractional initial value problem (FIVP) with a smooth source term. As such, the singularity of the new basis can be tailored to that of the singular solutions to a class of time-fractional PDEs, leading to spectrally accurate approximation. It also provides the acceptable solution to more general singular problems.

Keywords Fractional differential equations · Generalised Birkhoff interpolation · Nonstandard singular basis functions

Mathematics Subject Classification 41A05 · 41A10 · 41A25 · 65M70 · 65N35

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1 Introduction

The usual spectral method using classical orthogonal polynomials as basis functions enjoys high accuracy for problems with smooth solutions (see, e.g., [3, 13, 41] and the references therein). However, its fidelity and accuracy can be deleteriously degraded when the solutions exhibit locally singular behaviours. The singularities may occur in various scenarios such as PDEs in non-smooth computational domains with corners, with discontinuous coefficients, or with nonlocal operators involving singular kernels/weights. For a long time, mathematical and numerical study of singular problems has been a longstanding subject attracting much research interest. In recent years, intensive research efforts have been devoted to numerical solution of fractional PDEs (see, e.g., [9, 10, 22, 28, 33, 34, 45, 47] for finite difference or finite element methods, [6, 25–27, 54] for spectral methods, and many references therein). It is noteworthy that the usual polynomial-based spectral methods (e.g., in the pioneer works [25, 26]) cannot really resolve the numerical challenges of the (i) singularity and (ii) non-locality induced by the fractional integral/derivative operators. We therefore feel compelled to highlight some recent attempts in dealing with these two numerical issues, but with emphasis on spectral algorithms using non-standard basis functions.

(a) *Jacobi poly-fractonomials* (*JPFs*) *and generalised Jacobi functions* (*GJFs*) As a remarkable advancement, Zayernouri and Karniadakis [54] introduced the so-called JPFs defined as eigenfunctions of some fractional Sturm-Liouville operator. The JPFs are non-polynomial singular basis functions possessing attractive fractional calculus properties, which can lead to sparse linear systems and spectrally accurate solution of certain class of fractional PDEs. Notably, the JPFs (up to some constants) are identical to special families of GJFs first introduced in [14]. The recent work [6] significantly enriched the applications of GJFs to fractional PDEs, and more importantly provided a rigorous error analysis in the fractional context. It is also worthwhile to mention the interesting developments along this line [18, 19, 23, 30, 40, 52, 53, 58]. However, such approaches usually work well for some specific types of end point (or corner) singularities.

(b) *Müntz polynomials* In contrast to the algebraic polynomials, the Müntz polynomials are of the form: $\sum_{k=0}^{n} a_k x^{\lambda_k}$ with real $\{a_k\}$ (note: they are dense in $L^2(0,1)$, if and only if, $\lambda_0 + \sum_{k=1}^{\infty} \lambda_k^{-1} = \infty$ for $0 \le \lambda_0 < \lambda_1 < \cdots$). With *a priori* knowledge of the singularity of the underlying solution, such a tool can provide very accurate approximation to a large class of singular problems with suitable choices of $\{\lambda_k\}$ (see, e.g., [2, 35, 36]). Recently, Shen and Wang [43] associated the Müntz polynomials with Jacobi polynomials and developed efficient and accurate Müntz-Galerkin methods for some singular problems with typical singularities of the type: $\lambda_k = \alpha k$ with $\alpha \in (0,1)$. Hou and Xu [17] further studied the so-called factional Jacobi polynomials: $J_n^{\alpha,\beta,\lambda}(x) = J_n^{\alpha,\beta}(2x^\lambda - 1)$ for $x \in (0,1), \alpha, \beta > -1$ and $\lambda > 0$, with applications to the integral-differential and fractional differential equations.

(c) *Enriched spectral methods* A second approach to deal with singular problems is to add some special shape functions (to capture local singularities or treat certain solution structures) to the usual polynomial basis, as with the finite element methods (cf. [1]). A hybrid collocation method enriched with spectral singular functions to fit leading singularity was studied in [4]. The very recent work [16] proposed enriched spectral methods to resolve boundary or inner layers. Moreover, Chen and Shen [5] developed efficient enriched spectral methods for a more general class of singular problems. In addition, the enriched technique turned out to be very essential for accurate solutions of the Maxwell equations with Cole-Cole media in [20].

In this paper, we intend to introduce new singular basis functions for time-fractional PDEs from a very different perspective. More precisely, we consider some prototypical fractional initial value problem with a smooth source term $f(x)$ (which can be well approximated by polynomials). By taking $f(x)$ to be the interpolating basis functions, we directly invert the fractional IVP (together with the initial values) and then define the new singular basis from the inverse operator acting upon the interpolation basis. We propose fast recursive formulas for computing the so-defined basis functions and the associated fractional collocation matrices, which can actually be pre-computed. It is noteworthy that the main idea for such a construction is inspired from the design of well-conditioned collocation methods using the notion of the Birkhoff interpolation (cf. [7, 19, 32, 48, 56, 57]). Here, we also estimate the interpolation error of this type of the generalised Birkhoff interpolation and demonstrate that the new approach can provide very accurate approximation to a class of time-fractional PDEs with smooth source terms.

2 Preliminaries

In this section, we make necessary preparations for the exposition of the algorithm and analysis. We first recap on a useful solution formula of a prototype fractional initial-valued equation with a Caputo fractional derivative (FIVP). We then collect some relevant properties of the involved Mittag-Leffler (ML) functions. Finally, we review some related properties of Jacobi polynomials and Jacobi-Gauss-Lobatto (JGL) interpolation.

Let $\mathbb{N}$ and $\mathbb{R}$ be the sets of positive integers and real numbers, respectively, and denote

$$\mathbb{N}_0 := \{0\} \cup \mathbb{N}, \quad \mathbb{R}^+ := \big\{a \in \mathbb{R} : a > 0\big\}, \quad \mathbb{R}_0^+ := \{0\} \cup \mathbb{R}^+. \tag{1}$$

The following definition of the Riemann-Liouville fractional integral and Caputo fractional derivative can be found from many resources (see, e.g., [8, 37]). For $\rho \in \mathbb{R}^+$, the left-sided and right-sided fractional integrals of order ρ are defined by

$$({}_aI_t^\rho u)(t) = \frac{1}{\Gamma(\rho)} \int_a^t \frac{u(\tau)}{(t-\tau)^{1-\rho}} \mathrm{d}\tau; \quad ({}_tI_b^\rho u)(t) = \frac{1}{\Gamma(\rho)} \int_t^b \frac{u(\tau)}{(\tau-t)^{1-\rho}} \mathrm{d}\tau, \tag{2}$$

for $t \in (a,b)$, respectively, where $\Gamma(\cdot)$ is the Gamma function. For $\mu \in (k-1,k)$ with $k \in \mathbb{N}$, the left-sided Caputo fractional derivative of order μ is defined by

$$\big({}_a^C D_t^\mu \, u\big)(t) = {}_aI_t^{k-\mu} \, \big(D^k u\big)(t) = \frac{1}{\Gamma(k-\mu)} \int_a^t \frac{D^k u(\tau)}{(t-\tau)^{\mu-k+1}} \mathrm{d}\tau, \tag{3}$$

where $D^k = \frac{\mathrm{d}^k}{\mathrm{d}t^k}$ is the ordinary derivative. Similarly, we can define the right-sided Caputo fractional derivative.

Note that ${}_a^C D_t^k = D^k$, if $\mu = k \in \mathbb{N}$. Recall that (see, e.g., [8, P. 49]): for $\nu \in (k-1,k)$ with $k \in \mathbb{N}$,

$${}_{-1}^{\,C}D_t^\nu (t+1)^\alpha = \begin{cases} 0, & \text{if} \quad \alpha \in \{0,1,\dots,k-1\}, \\ \dfrac{\Gamma(\alpha+1)}{\Gamma(\alpha-\nu+1)}(t+1)^{\alpha-\nu}, & \text{if} \quad \alpha > k-1, \quad \alpha \in \mathbb{R}. \end{cases} \tag{4}$$

However, there is no explicit and compact formula for $-1 < \alpha < k-1$ and $\alpha \notin \mathbb{N}$.

2.1 FIVPs and Mittag-Leffler Functions

The following solution formulas of FIVPs (cf. [37]) play an important part in our algorithm development.

Lemma 2.1 *Consider the FIVP: for $\mu \in (k-1, k)$ with $k \in \mathbb{N}$,*

$$\begin{aligned} &\mathscr{L}_{\mu,\lambda}[u](t) := {}_a^C D_t^{\mu} u(t) + \lambda\, u(t) = f(t), \quad t \in (a, b], \\ &u^{(l)}(a) = u_{0,l}, \quad l = 0, \ldots, k-1, \end{aligned} \tag{5}$$

where the constant $\lambda \in \mathbb{R}_0^+$ and f is a given integrable function. Then its solution is given by

$$\begin{aligned} u(t) &= \mathscr{L}_{\mu,\lambda}^{-1}\big[f; \{u_{0,l}\}_{l=0}^{k-1}\big](t) \\ &= \sum_{l=0}^{k-1} e_{\mu,l+1}(t-a;\lambda)\, u_{0,l} + \int_a^t e_{\mu,\mu}(t-\tau;\lambda) f(\tau)\, \mathrm{d}\tau, \end{aligned} \tag{6}$$

which involves the Mittag-Leffler (ML) functions with two parameters defined by

$$e_{\alpha,\beta}(z;\lambda) := z^{\beta-1} E_{\alpha,\beta}(-\lambda z^{\alpha}), \quad E_{\alpha,\beta}(z) := \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + \beta)}, \quad \alpha, \beta > 0. \tag{7}$$

Remark 2.1 The so-defined $e_{\alpha,\beta}(z;\lambda)$ is called the generalised ML function, and its Laplace transform is given by the explicit formula (cf. [12]):

$$\mathcal{L}[e_{\alpha,\beta}](s) = \int_0^{\infty} \mathrm{e}_{\alpha,\beta}(t;\lambda) \mathrm{e}^{-st}\, \mathrm{d}t = \frac{s^{\alpha-\beta}}{s^{\alpha} + \lambda}, \tag{8}$$

for $\alpha, \beta, \lambda > 0$.

In what follows, we shall use the following property of a singular integral involving the ML function as the kernel function.

Lemma 2.2 *For $\lambda > 0$ and $\mu \in (k-1, k)$ with $k \in \mathbb{N}$, we define*

$$u(t) := \int_0^t e_{\mu,\mu}(t-\tau;\lambda) f(\tau)\, \mathrm{d}\tau, \quad t > 0, \tag{9}$$

where f is a given integrable function. Then we have

$${}_0^C D_t^{\nu} u(t) = \int_0^t e_{\mu,\mu-\nu}(t-\tau;\lambda) f(\tau)\, \mathrm{d}\tau, \tag{10}$$

where $\nu \in (0, \mu]$.

Proof Let $F(s) := \mathcal{L}[f(t)]$. Using the convolution property of the Laplace transform and (8) with $\alpha = \beta = \mu$, we have

$$\mathcal{L}[u](s) = \mathcal{L}[e_{\mu,\mu} * f](s) = \frac{F(s)}{s^\mu + \lambda}. \tag{11}$$

We find that for $\nu \in (0, \mu]$ and $\nu \in (m, m+1]$ (see, e.g., [37, P. 106])

$$\mathcal{L}\left[{}_0^C D_t^\nu u\right](s) = s^\nu \mathcal{L}\left[u(t)\right](s) - \sum_{k=0}^{m} s^{\nu-k-1} u^{(k)}(0) = \frac{s^\nu}{s^\mu + \lambda} F(s),$$

which yields

$${}_0^C D_t^\nu u(t) = \mathcal{L}^{-1}\left[\frac{s^\nu}{s^\mu + \lambda} F(s)\right] = \int_0^t e_{\mu,\mu-\nu}(t-\tau;\lambda) f(\tau)\,\mathrm{d}\tau.$$

This completes the proof.

2.2 Jacobi Polynomials

Let $P_n^{(\alpha,\beta)}(x)$ be the Jacobi polynomial of degree n with $\alpha, \beta > -1$ defined on $\Lambda = (-1, 1)$. The Jacobi polynomials are defined by the three-term recurrence (cf. [46]):

$$\begin{aligned} &P_{n+1}^{(\alpha,\beta)}(x) = \left(a_n^{(\alpha,\beta)} x - b_n^{(\alpha,\beta)}\right) P_n^{(\alpha,\beta)}(x) - c_n^{(\alpha,\beta)} P_{n-1}^{(\alpha,\beta)}(x), \quad n \geq 1, \\ &P_0^{(\alpha,\beta)}(x) = 1, \quad P_1^{(\alpha,\beta)}(x) = \frac{1}{2}(\alpha+\beta+2)x + \frac{1}{2}(\alpha-\beta), \end{aligned} \tag{12}$$

where

$$a_n^{(\alpha,\beta)} = \frac{(2n+\alpha+\beta+1)(2n+\alpha+\beta+2)}{2(n+1)(n+\alpha+\beta+1)}, \tag{13a}$$

$$b_n^{(\alpha,\beta)} = \frac{(\beta^2-\alpha^2)(2n+\alpha+\beta+1)}{2(n+1)(n+\alpha+\beta+1)(2n+\alpha+\beta)}, \tag{13b}$$

$$c_n^{(\alpha,\beta)} = \frac{(n+\alpha)(n+\beta)(2n+\alpha+\beta+2)}{(n+1)(n+\alpha+\beta+1)(2n+\alpha+\beta)}. \tag{13c}$$

We have

$$P_n^{(\alpha,\beta)}(-1) = (-1)^n P_n^{(\beta,\alpha)}(1), \; P_n^{(\alpha,\beta)}(1) = \frac{\Gamma(n+\alpha+1)}{n!\Gamma(\alpha+1)}. \tag{14}$$

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

$$\int_{-1}^{1} P_n^{(\alpha,\beta)}(x) P_m^{(\alpha,\beta)}(x) \omega^{(\alpha,\beta)}(x)\,\mathrm{d}x = \gamma_n^{(\alpha,\beta)} \delta_{mn}, \tag{15}$$

where δ_{mn} is the Kronecker symbol, and

$$\gamma_n^{(\alpha,\beta)} = \frac{2^{\alpha+\beta+1}\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}{(2n+\alpha+\beta+1)n!\,\Gamma(n+\alpha+\beta+1)}. \tag{16}$$

In what follows, we shall use the Jacobi-Gauss-Radau (JGR) interpolation and quadrature. Let $x_0 = -1$ and $\{x_j\}_{j=1}^N$ be the zeros of $P_N^{\alpha,\beta+1}(x)$, and let $\{\omega_j\}_{j=0}^N$ be the corresponding weights (cf. [41, Thm. 3.26]). Then, the JGR quadrature has the exactness

$$\int_{-1}^{1} p(x)\omega^{(\alpha,\beta)}(x)\mathrm{d}x = \sum_{j=0}^{N} p(x_j)\omega_j, \quad \forall p \in \mathcal{P}_{2N},$$

where $\mathcal{P}_N$ denotes the set of all polynomials of degree less than or equal to N.

3 Generalised Birkhoff Interpolation and New Basis Functions

In this section, we aim at developing spectrally accurate numerical algorithms for FIVPs with smooth source terms. Following the spirit of [48, 49], we introduce a generalised Birkhoff interpolation that interpolates $\mathscr{L}_{\mu,\lambda}[u]$ in (5) at "interior" JGR points, which leads to new non-polynomial basis functions for the efficient spectral algorithms.

3.1 New Basis Functions for FIVPs with $\mu \in (0,1)$

To show the essential idea, we first consider $\mathscr{L}_{\mu,\lambda}$ with $\mu \in (0,1)$.

Given a function u on $\bar{\Lambda}$ such that $\mathscr{L}_{\mu,\lambda}[u] \in C(\bar{\Lambda})$, consider the Birkhoff-type interpolation problem: find $q \in \mathcal{Q}_N$ (a finite-dimensional space to be specified later) such that

$$\mathscr{L}_{\mu,\lambda}[q](x_i) = \mathscr{L}_{\mu,\lambda}[u](x_i), \quad 1 \le i \le N; \quad q(x_0) = u(x_0), \tag{17}$$

where $\{x_i\}_{i=0}^N$ (with $x_0 = -1$) are the JGR points.

Different from Lagrange, Hermite and usual Birkhoff interpolations (cf. [29, 44]), the interplant q agrees with u in the operator sense at interior interpolating points in this context. In fact, there are various ways to select the space $\mathcal{Q}_N$. Here, our choice is based upon the assumption that $\mathcal{L}_{\mu,\lambda}[u]$ is smooth and can be well approximated by polynomials. More precisely, we choose $\mathcal{Q}_N$ such that

$$\mathscr{L}_{\mu,\lambda}[q] \in \mathcal{P}_{N-1}, \quad \forall\, q \in \mathcal{Q}_N. \tag{18}$$

Let $\{\hbar_j\}_{j=1}^N$ be the Lagrange interpolating basis polynomials associated with the interior JGR points $\{x_j\}_{j=1}^N$ (exclusive of $x_0 = -1$), i.e.,

$$\hbar_j \in \mathcal{P}_{N-1}, \quad \hbar_j(x_i) = \delta_{ij}, \quad 1 \le i,j \le N. \tag{19}$$

In view of (18), we have

$$\mathscr{L}_{\mu,\lambda}[q](x) = \sum_{j=1}^{N} \mathscr{L}_{\mu,\lambda}[u](x_j)\hbar_j(x). \tag{20}$$

Solving the FIVP: (20), together with the initial condition: $q(-1) = u(-1)$, we obtain from Lemma 2.1 that the interplant of u is given by

$$q(x) = u(-1)e_{\mu,1}(1+x;\lambda) + \sum_{j=1}^{N} \mathscr{L}_{\mu,\lambda}[u](x_j) \int_{-1}^{x} e_{\mu,\mu}(x-y;\lambda)\, \hbar_j(y)\,\mathrm{d}y. \tag{21}$$

Formally, we define the generalised interpolation:

$$\left(\mathcal{I}_N^{\mu,\lambda} u\right)(x) := u(-1)Q_0^{\mu}(x) + \sum_{j=1}^{N} \mathscr{L}_{\mu,\lambda}[u](x_j) Q_j^{\mu}(x), \tag{22}$$

where the generalised interpolating basis functions are

$$Q_0^{\mu}(x) := Q_0^{\mu}(x;\lambda) = e_{\mu,1}(1+x;\lambda), \tag{23}$$

$$Q_j^{\mu}(x) := Q_j^{\mu}(x;\alpha,\beta,\lambda) = \int_{-1}^{x} e_{\mu,\mu}(x-y;\lambda)\, \hbar_j(y)\,\mathrm{d}y, \quad 1 \le j \le N. \tag{24}$$

In fact, we can show readily that the so-defined $\{Q_j^{\mu}\}$ with $\mu \in (0,1)$ satisfy $\mathscr{L}_{\mu,\lambda}[Q_j^{\mu}] \in \mathcal{P}_{N-1}$, and the interpolating conditions

$$\begin{aligned} &Q_0^{\mu}(-1) = 1, \quad \mathscr{L}_{\mu,\lambda}[Q_0^{\mu}](x_i) = 0, \quad 1 \le i \le N;\\ &Q_j^{\mu}(-1) = 0, \quad 1 \le j \le N; \quad \mathscr{L}_{\mu,\lambda}[Q_j^{\mu}](x_i) = \delta_{ij}, \quad 1 \le i,j \le N. \end{aligned} \tag{25}$$

Indeed, we deduce from Lemma 2.1 and (23)–(24) that

$$\mathscr{L}_{\mu,\lambda}[Q_0^{\mu}](x) = 0, \;\; Q_0^{\mu}(-1) = 1; \quad \mathscr{L}_{\mu,\lambda}[Q_j^{\mu}](x) = \hbar_j(x), \;\; Q_j^{\mu}(-1) = 0, \;\; 1 \le j \le N. \tag{26}$$

This implies (25). It is evident that $\mathscr{L}_{\mu,\lambda}[Q_j^{\mu}] \in \mathcal{P}_{N-1}$, and $\{Q_j^{\mu}\}$ are linearly independent.

In view of the above, we call $\{Q_j^{\mu}\}_{j=0}^{N}$ the generalised Birkhoff interpolating basis of (17)–(18), and $\mathcal{I}_N^{\mu,\lambda}$ is the corresponding generalised Birkhoff interpolating operator.

3.2 Extension of the New Basis Functions to $\mu \in (1,2)$

It is straightforward to extend the generalised Birkhoff interpolation in (17) with $\mu \in (0,1)$ to $\mu \in (1,2)$. Accordingly, we consider the generalised Birkhoff interpolation: given a function $u \in C^1[-1,1)$ such that $\mathscr{L}_{\mu,\lambda}[u] \in C[-1,1)$ with $\mu \in (1,2)$, find $q \in \mathcal{Q}_{N+1}$ (to be specified later) such that

$$\mathscr{L}_{\mu,\lambda}[q](x_i) = \mathscr{L}_{\mu,\lambda}[u](x_i), \quad 1 \le i \le N; \quad q(-1) = u(-1), \quad q'(-1) = u'(-1), \tag{27}$$

where $\{x_j\}_{j=0}^{N}$ (with $x_0 = -1$) are the JGR points with parameters $\alpha, \beta > -1$. As before, we choose $\mathcal{Q}_{N+1}$ such that

$$\mathscr{L}_{\mu,\lambda}[q] \in \mathcal{P}_{N-1}, \quad \forall\, q \in \mathcal{Q}_{N+1}. \tag{28}$$

Like (20), we write

$$\mathscr{L}_{\mu,\lambda}[q](x) = \sum_{j=1}^{N} \mathscr{L}_{\mu,\lambda}[u](x_j)\hbar_j(x), \quad q^{(k)}(-1) = u^{(k)}(-1), \;\; k = 0,1, \tag{29}$$

where $\{\hbar_j\}$ are the same as in (19). Then, by Lemma 2.1, the interplant of u is given by

$$q(x) = u(-1)Q_0^{\mu}(x) + u'(-1)Q_{-1}^{\mu}(x) + \sum_{j=1}^{N} \mathscr{L}_{\mu,\lambda}[u](x_j)Q_j^{\mu}(x), \tag{30}$$

where

$$Q_{-1}^{\mu}(x) := Q_{-1}^{\mu}(x;\lambda) = e_{\mu,2}(1+x;\lambda), \quad Q_0^{\mu}(x) := Q_{-1}^{\mu}(x;\lambda) = e_{\mu,1}(1+x;\lambda), \tag{31}$$

$$Q_j^{\mu}(x) := Q_j(x;\alpha,\beta,\lambda) = \int_{-1}^{x} e_{\mu,\mu}(x-y;\lambda)\, \hbar_j(y)\,\mathrm{d}y, \quad 1 \le j \le N. \tag{32}$$

Then we define the generalised interpolation operator:

$$\big(\mathcal{I}_N^{\mu,\lambda} u\big)(x) = u'(-1)\, Q_{-1}^{\mu}(x) + u(-1)\, Q_0^{\mu}(x) + \sum_{j=1}^{N} \mathscr{L}_{\mu,\lambda}[u](x_j)\, Q_j^{\mu}(x). \tag{33}$$

As before, we can verify readily that $\mathscr{L}_{\mu,\lambda}[Q_j^{\mu}] \in \mathcal{P}_{N-1}$, and the interpolating basis satisfies the interpolation conditions:

$$\begin{aligned}
&Q_{-1}^{\mu}(-1) = 0, \quad \frac{\mathrm{d}}{\mathrm{d}x} Q_{-1}^{\mu}(-1) = 1, \quad \mathscr{L}_{\mu,\lambda}[Q_{-1}^{\mu}](x_i) = 0, \quad 1 \le i \le N;\\
&Q_0^{\mu}(-1) = 1, \quad \frac{\mathrm{d}}{\mathrm{d}x} Q_0^{\mu}(-1) = 0, \quad \mathscr{L}_{\mu,\lambda}[Q_0^{\mu}](x_i) = 0, \quad 1 \le i \le N;\\
&Q_j^{\mu}(-1) = \frac{\mathrm{d}}{\mathrm{d}x} Q_j^{\mu}(-1) = 0, \quad 1 \le j \le N, \quad \mathscr{L}_{\mu,\lambda}[Q_j^{\mu}](x_i) = \delta_{ij}, \ \ 1 \le i,j \le N.
\end{aligned} \tag{34}$$

3.3 Computing the New Basis and the Related Fractional Differentiation Matrices

Our starting point is to show that $\{\hbar_j\}_{j=1}^{N}$ in (19) has the following representation.

Lemma 3.1 *Let $\{x_j, \omega_j\}_{j=0}^{N}$ with $x_0 = -1$ be the JGR points and quadrature weights. Then we have*

$$\hbar_j(x) = \sum_{n=0}^{N-1} \xi_{nj} P_n^{(\alpha,\beta)}(x), \quad 1 \le j \le N, \tag{35}$$

where

$$\xi_{nj} = \frac{1}{\gamma_n^{(\alpha,\beta)}} \left\{ -\frac{P_N^{(\alpha,\beta+1)}(-1)}{(1+x_j)\frac{\mathrm{d}}{\mathrm{d}x} P_N^{(\alpha,\beta+1)}(x_j)} P_n^{(\alpha,\beta)}(-1)\omega_0 + P_n^{(\alpha,\beta)}(x_j)\omega_j \right\}. \tag{36}$$

Proof By the exactness of JGR quadrature, we have

$$\begin{aligned}
\xi_{nj} &= \frac{1}{\gamma_n^{(\alpha,\beta)}} \int_{-1}^{1} \hbar_j(x) P_n^{(\alpha,\beta)}(x) \omega^{(\alpha,\beta)}(x)\mathrm{d}x = \frac{1}{\gamma_n^{(\alpha,\beta)}} \sum_{i=0}^{N} \hbar_j(x_i) P_n^{(\alpha,\beta)}(x_i)\omega_i \\
&= \frac{1}{\gamma_n^{(\alpha,\beta)}} \big\{ \hbar_j(-1) P_n^{(\alpha,\beta)}(-1)\omega_0 + P_n^{(\alpha,\beta)}(x_j)\omega_j \big\}, \quad 1 \le j \le N.
\end{aligned} \tag{37}$$

Now, we evaluate $\hbar_j(-1)$. Since $\{\hbar_j\}$ are associated with the interpolating points $\{x_j\}_{j=1}^N$, which are zeros of $P_N^{(\alpha,\beta+1)}(x)$, we have the representation:

$$\hbar_j(x) = \frac{P_N^{(\alpha,\beta+1)}(x)}{(x-x_j)\frac{\mathrm{d}}{\mathrm{d}x}P_N^{(\alpha,\beta+1)}(x_j)}, \quad 1 \le j \le N. \tag{38}$$

This leads to the desired formula.

We now introduce efficient algorithms for computing the new basis, and the associated differentiation matrix $\{{}_{-1}^{C}D_x^{\nu}Q_j^{\mu}\}_{j=1}^N$ for $\nu \in [0,\mu]$ and $\mu \in (0,2)$. Thanks to (24) and (35), the computation of $\{Q_j^{\mu}\}_{j=1}^N$ boils down to evaluating

$$\phi_n^{\mu}(x) := \phi_n^{\mu}(x;\alpha,\beta,\lambda) = \int_{-1}^{x} e_{\mu,\mu}(x-y;\lambda)\, P_n^{(\alpha,\beta)}(y)\,\mathrm{d}y, \quad x \in (-1,1), \tag{39}$$

for $\mu, \lambda > 0$ and real $\alpha, \beta > -1$. Likewise, the computation of $\{{}_{-1}^{C}D_x^{\nu}Q_j^{\mu}\}_{j=1}^N$ relies on the evaluation of $\{{}_{-1}^{C}D_x^{\nu}\phi_n^{\mu}\}_{n\ge 0}$.

The recursive algorithm builds upon the auxiliary function

$$\Phi_{m,n}^{\mu,\nu}(x) := \Phi_{m,n}^{\mu,\nu}(x;\alpha,\beta,\lambda) = {}_{-1}^{C}D_x^{\nu}\int_{-1}^{x} e_{\mu,\mu}(x-y;\lambda)\Big(\frac{1+y}{2}\Big)^m P_n^{(\alpha,\beta)}(y)\mathrm{d}y. \tag{40}$$

Apparently, we have

$$\phi_n^{\mu}(x) = \Phi_{0,n}^{\mu,0}(x), \quad {}_{-1}^{C}D_x^{\nu}\phi_n^{\mu}(x) = \Phi_{0,n}^{\mu,\nu}(x). \tag{41}$$

In Fig. 1, we provide a schematic illustration of the following "downwind" recursive algorithm for computing $\{{}_{-1}^{C}D_x^{\nu}\phi_n^{\mu} = \Phi_{0,n}^{\mu,\nu}\}_{n=0}^N$ (see the leftmost column in Fig. 1). In particular, for $\nu = 0$, we have $\{\phi_n^{\mu} = {}_{-1}^{C}D_x^{0}\phi_n^{\mu} = \Phi_{0,n}^{\mu,0}\}_{n=0}^N$.

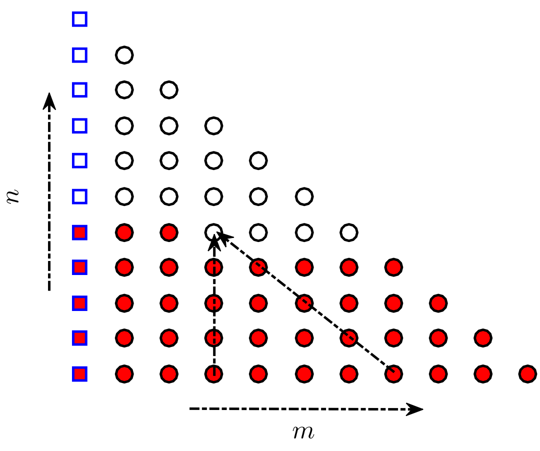


Fig. 1 Diagram for computing $\{{}_{-1}^{C}D_x^{\nu}\phi_n^{\mu} = \Phi_{0,n}^{\mu,\nu}\}_{n=0}^N$ (marked by "□") with $N = 10$, where the stencils marked by "○" are marched by (44)

Proposition 3.1 *With a pre-computation of*

$$\Phi^{\mu,\nu}_{m,0}(x) = 2^{-m} m!\, e_{\mu,\mu-\nu+m+1}(1+x;\lambda), \quad 0 \le m \le N, \tag{42}$$

and

$$\Phi^{\mu,\nu}_{m,1}(x) = (\alpha+\beta+2)\Phi^{\mu,\nu}_{m+1,0}(x) - (\beta+1)\Phi^{\mu,\nu}_{m,0}(x), \quad 0 \le m \le N-1, \tag{43}$$

we can compute $\{ {}_{-1}^{C}D_x^{\nu}\phi_n^{\mu}\}$ in (41) *with* $1 \le n \le N-1$, *by the "downwind" recurrence relation*:

$$\Phi^{\mu,\nu}_{m,n+1}(x) = 2a_n^{(\alpha,\beta)}\Phi^{\mu,\nu}_{m+1,n}(x) - \left(a_n^{(\alpha,\beta)} + b_n^{(\alpha,\beta)}\right)\Phi^{\mu,\nu}_{m,n}(x) - c_n^{(\alpha,\beta)}\Phi^{\mu,\nu}_{m,n-1}(x), \tag{44}$$

for $0 \le m \le N-m-1$, *where* $\left\{a_n^{(\alpha,\beta)}, b_n^{(\alpha,\beta)}, c_n^{(\alpha,\beta)}\right\}$ *are defined in* (13).

Proof Recall the following identity (cf. [11]): for $\lambda \in \mathbb{R}^+$ and $r > -1$, we obtain

$$\frac{1}{\Gamma(r+1)} \int_a^t e_{\mu,\nu}(t-\tau;\lambda)(\tau-a)^r \mathrm{d}\tau = e_{\mu,\nu+r+1}(t-a;\lambda), \quad t \in (a,b). \tag{45}$$

Then, we have from (40) that

$$\Phi^{\mu,\nu}_{m,0}(x) = 2^{-m} m!\, {}_{-1}^{C}D_x^{\nu} e_{\mu,\mu+m+1}(1+x;\lambda). \tag{46}$$

From (7), we find

$$\begin{aligned} e_{\mu,\mu+m+1}(1+x;\lambda) &= (1+x)^{\mu+m} \sum_{k=0}^{\infty} \frac{(-\lambda)^k (1+x)^{\mu k}}{\Gamma(\mu k+\mu+m+1)} \\ &= \sum_{k=0}^{\infty} \frac{(-\lambda)^k (1+x)^{\mu k+\mu+m}}{\Gamma(\mu k+\mu+m+1)}. \end{aligned}$$

Thus, we derive from (4) that

$$\begin{aligned} {}_{-1}^{C}D_x^{\nu} e_{\mu,\mu+m+1}(1+x;\lambda) &= \sum_{k=0}^{\infty} \frac{(-\lambda)^k \ {}_{-1}^{C}D_x^{\nu}(1+x)^{\mu k+\mu+m}}{\Gamma(\mu k+\mu+m+1)} \\ &= \sum_{k=0}^{\infty} \frac{(-\lambda)^k (1+x)^{\mu k+\mu+m-\nu}}{\Gamma(\mu k+\mu+m+1-\nu)} = e_{\mu,\mu-\nu+m+1}(1+x;\lambda). \end{aligned}$$

Therefore, we have

$$\Phi^{\mu,\nu}_{m,0}(x) = 2^{-m} m!\, e_{\mu,\mu-\nu+m+1}(1+x;\lambda), \quad 0 \le m \le N.$$

Using the explicit form of $P_1^{(\alpha,\beta)}$, we obtain

$$\begin{aligned}\Phi^{\mu,\nu}_{m,1}(x) &= {}_{-1}^{C}D_x^{\nu}\int_{-1}^{x} e_{\mu,\mu}(x-y;\lambda)\Big(\frac{1+y}{2}\Big)^m\Big(\frac{1}{2}(\alpha+\beta+2)y+\frac{1}{2}(\alpha-\beta)\Big)\,\mathrm{d}y\\ &= (\alpha+\beta+2)\Phi^{\mu,\nu}_{m+1,0}(x)-(\beta+1)\Phi^{\mu,\nu}_{m,0}(x).\end{aligned} \tag{47}$$

By the three-term recurrence relation (12) and the definition (40), we have

$$\begin{aligned}&\Phi^{\mu,\nu}_{m,n+1}(x)\\ &= {}_{-1}^{C}D_x^{\nu}\int_{-1}^{x} e_{\mu,\mu}(x-y;\lambda)\Big(\frac{1+y}{2}\Big)^m\Big\{\big(a_n^{(\alpha,\beta)}y-b_n^{(\alpha,\beta)}\big)P_n^{(\alpha,\beta)}(y)-c_n^{(\alpha,\beta)}P_{n-1}^{(\alpha,\beta)}(y)\Big\}\mathrm{d}y\\ &= 2a_n^{(\alpha,\beta)}\Phi^{\mu,\nu}_{m+1,n}(x)-\big(a_n^{(\alpha,\beta)}+b_n^{(\alpha,\beta)}\big)\Phi^{\mu,\nu}_{m,n}(x)-c_n^{(\alpha,\beta)}\Phi^{\mu,\nu}_{m,n-1}(x).\end{aligned} \tag{48}$$

This ends the proof.

For notational convenience, we introduce the matrices $\boldsymbol{Q}^{(\mu,\nu)}, \boldsymbol{\Xi}$ and $\boldsymbol{\Phi}^{(\mu,\nu)}$ with the entries

$$\big(\boldsymbol{Q}^{(\mu,\nu)}_{ij} = {}_{-1}^{C}D_x^{\nu}Q_j^{\mu}(x_i)\big)_{0\le i,j\le N},\quad \big(\Xi_{nj}=\xi_{nj}\big)_{0\le n\le N-1}^{0\le j\le N},\quad \big(\boldsymbol{\Phi}^{(\mu,\nu)}_{in}=\Phi^{\mu,\nu}_{0,n}(x_i)\big)_{0\le n\le N-1}^{0\le i\le N}. \tag{49}$$

Then from (24), (36), and (40)–(41), we obtain

$$\boldsymbol{Q}^{(\mu,\nu)} = \boldsymbol{\Phi}^{(\mu,\nu)}\,\boldsymbol{\Xi},\qquad \boldsymbol{Q}^{(\mu)} = \boldsymbol{\Phi}^{(\mu,0)}\,\boldsymbol{\Xi}, \tag{50}$$

where the matrix $\boldsymbol{Q}^{(\mu)}$ has the entries $\boldsymbol{Q}^{(\mu)}_{ij} = Q_j^{\mu}(x_i)$.

In Fig. 2, we plot several profiles of the new basis functions with $\mu = 0.5, 1.5$, associated with the Legendre and Chebyshev Gauss-Radau points. Indeed, the basis functions can fully capture the singularity of the solution to the special FIVP at $x = -1$.

4 Error Estimates of the Interpolation

In this section, we estimate the interpolation error of the generalised Birkhoff interpolation operator defined in (22) and (33).

Lemma 4.1 *For* $0 < \mu < 2$ *and* $\lambda > 0$, *we have*

$$\int_0^2 |e_{\mu,\mu}(x;\lambda)|\mathrm{d}x \le C, \tag{51}$$

where

$$C = \max\left\{\frac{1}{\lambda}\Big(1+\frac{C_2}{1+\lambda 2^{\mu}}\Big), C_1\Big(\big(1+\lambda 2^{\mu}\big)^{1/\mu}-1\Big)\frac{1}{\lambda}+\frac{C_2\ln(1+\lambda 2^{\mu})}{\lambda\mu}\right\}, \tag{52}$$

and C_1, C_2 *are given in* (53).

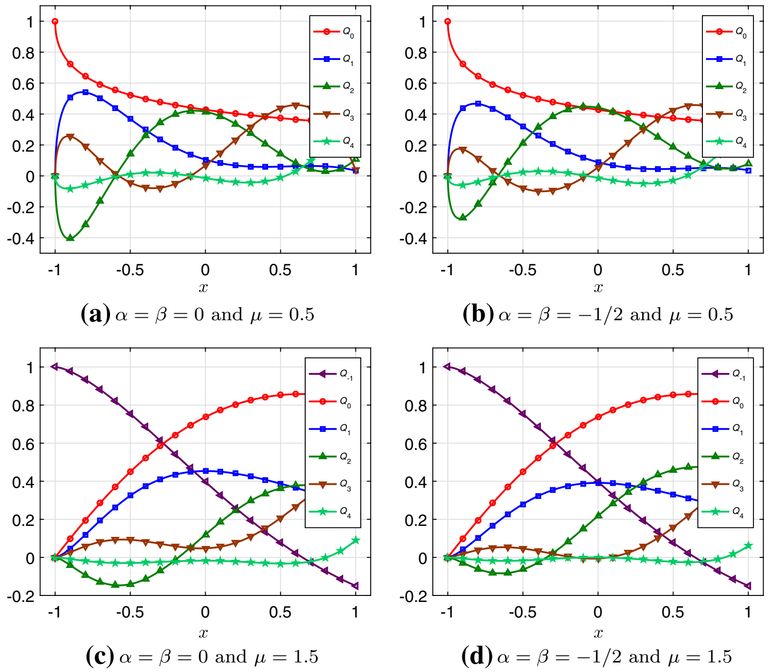


Fig. 2 Graphs of the new basis $\{Q_j^\mu\}$ with $\lambda=1$ and $N=4$

Proof In this proof, we shall use the following properties of the ML functions.

(i) For $\alpha<2$, $\beta\in\mathbb{R}$, and $\pi\alpha/2<\mu<\min\{\pi,\pi\alpha\}$, we have (see [37, Thm. 1.5]):

$$|E_{\alpha,\beta}(z)|\leq C_1\big(1+|z|\big)^{(1-\beta)/\alpha}\exp\big(\Re(z^{1/\alpha})\big)+\frac{C_2}{1+|z|},\quad |\arg(z)|\leq\mu, \tag{53}$$

where C_1 and C_2 are certain positive constants.

(ii) For $\lambda,\mu>0$ and positive integer m, we have (see [38, Lem. 3.2]):

$$\frac{\mathrm{d}^m}{\mathrm{d}t^m}E_{\mu,1}(-\lambda t^\mu)=-\lambda t^{\mu-m}E_{\mu,\mu-m+1}(-\lambda t^\mu),\quad t>0, \tag{54}$$

and

$$\frac{\mathrm{d}}{\mathrm{d}t}\big(tE_{\mu,2}(-\lambda t^\mu)\big)=E_{\mu,1}(-\lambda t^\mu),\quad t\geq 0. \tag{55}$$

(iii) For $0<\mu<1$, we have (see [38, Lem. 3.3]):

$$E_{\mu,\mu}(-t)\geq 0,\quad t\geq 0. \tag{56}$$

We first consider $\mu\in(0,1)$. From the above properties, we obtain

$$\begin{aligned}\int_0^\eta |e_{\mu,\mu}(x;\lambda)|\mathrm{d}x &= \int_0^\eta e_{\mu,\mu}(x;\lambda)\mathrm{d}x\\ &= -\frac{1}{\lambda}\int_0^\eta \frac{d}{\mathrm{d}t}E_{\mu,1}(-\lambda x^\mu)\mathrm{d}x = \frac{1}{\lambda}(1-E_{\mu,1}(-\lambda\eta^\mu))\\ &\le \frac{1}{\lambda}\Big(1+\frac{C_2}{1+\lambda\eta^\mu}\Big).\end{aligned} \tag{57}$$

This implies

$$\int_0^2 |e_{\mu,\mu}(x;\lambda)|\mathrm{d}x \le C, \quad \mu\in(0,1). \tag{58}$$

We now consider $\mu=1$. As $e_{1,1}(x;\lambda)=\exp(-\lambda x)$, we have

$$\int_0^\eta |e_{1,1}(x;\lambda)|\mathrm{d}x = -\frac{1}{\lambda}\int_0^\eta \frac{\mathrm{d}}{\mathrm{dx}}\exp(-\lambda x)\mathrm{d}x = \frac{1}{\lambda}(1-\exp(-\lambda\eta)) < \frac{1}{\lambda}. \tag{59}$$

Then we obtain

$$\int_0^2 |e_{1,1}(x;\lambda)|\mathrm{d}x \le C. \tag{60}$$

Finally, we consider $\mu\in(1,2)$. Using (53), we obtain

$$\begin{aligned}\int_0^2 |e_{\mu,\mu}(x;\lambda)|\mathrm{d}x &\le \int_0^2 \Big(x^{\mu-1}C_1\big(1+\lambda x^\mu\big)^{(1-\mu)/\mu}\exp\big(-\lambda^{1/\mu}x\big)+\frac{C_2x^{\mu-1}}{1+\lambda x^\mu}\Big)\mathrm{d}x\\ &\le \int_0^2 x^{\mu-1}C_1\big(1+\lambda x^\mu\big)^{(1-\mu)/\mu}\mathrm{d}x+\frac{C_2\ln(1+\lambda 2^\mu)}{\lambda\mu}\\ &= C_1\Big(\big(1+\lambda 2^\mu\big)^{1/\mu}-1\Big)\frac{1}{\lambda}+\frac{C_2\ln(1+\lambda 2^\mu)}{\lambda\mu} \le C,\end{aligned} \tag{61}$$

where

$$C=\max\left\{\frac{1}{\lambda}\Big(1+\frac{C_2}{1+\lambda 2^\mu}\Big),\ C_1\Big(\big(1+\lambda 2^\mu\big)^{1/\mu}-1\Big)\frac{1}{\lambda}+\frac{C_2\ln(1+\lambda 2^\mu)}{\lambda\mu}\right\}. \tag{62}$$

Clearly, we have $\lim\limits_{\lambda\to+\infty} C=0$. This completes the proof.

Here, we consider the class of functions satisfying the condition (see [50]) **AC)**: u is absolutely continuous up to $(m-1)$th derivative $u^{(m-1)}$ on $[-1,1]$ for some $m\ge 1$, and has the representation:

$$u^{(m-1)}(x) = u^{(m-1)}(-1) + \int_{-1}^{x} g(y)\mathrm{d}y, \tag{63}$$

where g is absolutely integrable and of bounded variation $\mathrm{Var}(g) < \infty$ on $[-1, 1]$. Define the norm as $V_m = \inf\{\mathrm{Var}(g)\}$ with all possible g satisfying (63).

We first consider the Gauss interpolation at the interior JGR points, i.e.,

$$\mathbb{I}_N^{(\alpha,\beta)} u(x) = \sum_{j=1}^{N} u(x_j)\hbar_j(x), \tag{64}$$

where $u \in C(-1, 1)$, and $\{\hbar_j\}$ are defined in (19).

Lemma 4.2 (see [50, Theorem 4.4]) *Suppose that $f(x)$ satisfies the condition* **AC).** *Then for $N \geq m + 1$ and $m \geq 1$,*

$$\|\mathbb{I}_N^{(\alpha,\beta)} f - f\|_{L^\infty(\Lambda)} \leq cN^{-m+\max\{0,\gamma-1/2\}} V_m, \tag{65}$$

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

With the above preparations, we are now ready to derive the main results on the generalised Birkhoff interpolation. By definition, we can rewrite them as

$$\left(\mathcal{I}_N^{\mu,\lambda} u\right)(x) = u(-1)Q_0^\mu(x) + \int_{-1}^{x} e_{\mu,\mu}(x-y;\lambda)\, \mathbb{I}_N^{(\alpha,\beta)}\left\{\mathscr{L}_{\mu,\lambda}[u](y)\right\} \mathrm{d}y, \quad \mu \in (0, 1), \tag{66}$$

and for $\mu \in (1, 2)$,

$$\left(\mathcal{I}_N^{\mu,\lambda} u\right)(x) = u'(-1)Q_{-1}^\mu(x) + u(-1)Q_0^\mu(x) + \int_{-1}^{x} e_{\mu,\mu}(x-y;\lambda)\, \mathbb{I}_N^{(\alpha,\beta)}\left\{\mathscr{L}_{\mu,\lambda}[u](y)\right\} \mathrm{d}y. \tag{67}$$

Theorem 4.1 *Suppose that $\mathscr{L}_{\mu,\lambda}[u]$ satisfies the condition* **AC).** *Then for $\mu \in (0, 2)$, $N \geq m + 1$ and $m \geq 1$, we have*

$$\left|\left(\mathcal{I}_N^{\mu,\lambda} u - u\right)(x)\right| \leq cN^{-m+\max\{0,\gamma-1/2\}} V_m, \quad x \in \bar{\Lambda}, \tag{68}$$

where $\gamma = \max\{\alpha, \beta + 1\}$, and c is a positive constant independent of u, N and m.

Proof For $\mu \in (0, 1)$, it is evident that by the definition (66),

$$\left(\mathcal{I}_N^{\mu,\lambda} u - u\right)(x) = \int_{-1}^{x} e_{\mu,\mu}(x-y;\lambda)\left\{\mathbb{I}_N^{(\alpha,\beta)}\left(\mathscr{L}_{\mu,\lambda}[u](y)\right) - \mathscr{L}_{\mu,\lambda}[u](y)\right\} \mathrm{d}y. \tag{69}$$

From Lemmas 4.2 and 4.1, we have

$$
\begin{aligned}
|\big(\mathcal{I}_N^{\mu,\lambda} u - u\big)(x)| &\le \Big\{ \int_{-1}^{x} |e_{\mu,\mu}(x-y;\lambda)| \mathrm{d}y \Big\} \big\| \mathbb{I}_N^{(\alpha,\beta)}(\mathscr{L}_{\mu,\lambda}[u]) - \mathscr{L}_{\mu,\lambda}[u] \big\|_{L^\infty(\Lambda)} \\
&= \Big\{ \int_{0}^{x+1} |e_{\mu,\mu}(y;\lambda)| \mathrm{d}y \Big\} \big\| \mathbb{I}_N^{(\alpha,\beta)}(\mathscr{L}_{\mu,\lambda}[u]) - \mathscr{L}_{\mu,\lambda}[u] \big\|_{L^\infty(\Lambda)} \\
&\le C \big\| \mathbb{I}_N^{(\alpha,\beta)}(\mathscr{L}_{\mu,\lambda}[u]) - \mathscr{L}_{\mu,\lambda}[u] \big\|_{L^\infty(\Lambda)} \le c N^{-m+\max\{0,\gamma-1/2\}} \, V_m.
\end{aligned}
\tag{70}
$$

This completes the proof.

As a simple application of the above interpolation estimates, we consider the model FIVP (5) with $\mu \in (0,1)$. Let $\{t_j\}$ be the JGR points as before. The scheme is to find $u_N \in \mathrm{spn}\{Q_j^\mu : 1 \le j \le N\}$ such that

$$
\begin{aligned}
\mathscr{L}_{\mu,\lambda}[u_N](t_j) &:= {}_a^C D_t^\mu u_N(t_j) + \lambda\, u_N(t_j) = f(t_j), \quad 1 \le j \le N, \\
u_N(a) &= u_0,
\end{aligned}
\tag{71}
$$

where $a = -1$. We infer from (6) that

$$
u_N(t_j) = e_{\mu,1}(t_j - a;\lambda)\, u_0 + \int_{-1}^{t_j} e_{\mu,\mu}(t_j - \tau;\lambda)\, \mathbb{I}_N^{(\alpha,\beta)} f(\tau)\, \mathrm{d}\tau,
\tag{72}
$$

and

$$
u_N(t_j) - u(t_j) = \int_{-1}^{t_j} e_{\mu,\mu}(t_j - \tau;\lambda) \big\{ \mathbb{I}_N^{(\alpha,\beta)} f(\tau) - f(\tau) \big\}\, \mathrm{d}\tau.
\tag{73}
$$

Then we deduce from Theorem 4.1 and its proof that

$$
\max_{0 \le j \le N} |u_N(t_j) - u(t_j)| \le c N^{-m+\max\{0,\gamma-1/2\}} \, V_m,
\tag{74}
$$

if f satisfies the condition **AC)**.

5 Some Applications and Numerical Results

In this section, we discuss the applications of spectral approximations using the nonstandard basis functions introduced in Section 3.

5.1 Fractional Initial Value Problems

We first consider the FIVP:

$$
{}_0^C D_t^\mu v(t) + a(t) v(t) = f(t), \quad t \in (0, T],
\tag{75}
$$

with the coefficient a being continuous on $[0, T]$, and the initial conditions

$$
v(0) = g_0 \quad \text{for} \quad \mu \in (0,1) \quad \text{or} \quad v(0) = g_0, \;\; v'(0) = g_1 \quad \text{for} \quad \mu \in (1,2).
\tag{76}
$$

For convenience, we transform the interval of interest to the reference interval $(-1, 1)$ via

$$t = \frac{1+x}{2}T, \quad u(x) = v(t), \quad b(x) = a(t), \quad h(x) = f(t).$$

Then, we can convert (75) into

$$\left(\frac{2}{T}\right)^{\mu} {}_{-1}^{C}D_x^{\mu} u(x) + b(x)u(x) = h(x), \quad x \in (-1, 1], \tag{77}$$

with the corresponding initial conditions:

$$u(-1) = g_0 \quad \text{for} \quad \mu \in (0,1) \quad \text{or} \quad u(-1) = g_0, \quad u'(-1) = Tg_1/2 \quad \text{for} \quad \mu \in (1,2).$$

For $\mu \in (0, 1)$, we employ the new basis $\{Q_j^{\mu}\}$ for (77), and look for the approximation of $u(x)$ as

$$u_N(x) = g_0\, Q_0^{\mu}(x) + \sum_{j=1}^{N} \tilde{v}_j\, Q_j^{\mu}(x),$$

satisfying

$$\left(\frac{2}{T}\right)^{\mu} {}_{-1}^{C}D_x^{\mu} u_N(x_j) + b(x_j)u_N(x_j) = h(x_j), \quad j = 1, \dots, N. \tag{78}$$

The linear system of (78) is

$$\left\{\boldsymbol{I}_N + \left(\left(\frac{T}{2}\right)^{\mu} \boldsymbol{\Lambda}_b - \lambda\right)\boldsymbol{Q}_{\text{in}}^{\mu}\right\} \tilde{\boldsymbol{v}} = \left(\frac{T}{2}\right)^{\mu} \boldsymbol{h} - g_0 \tilde{\boldsymbol{v}}_-, \tag{79}$$

where $\boldsymbol{I}_N$ is the identity matrix of order N,

$$\boldsymbol{\Lambda}_b = \text{diag}(b(x_1), b(x_2), \dots, b(x_N)), \quad \tilde{\boldsymbol{v}} = (\tilde{v}_1, \tilde{v}_2, \dots, \tilde{v}_N)^{\mathrm{T}}, \quad \boldsymbol{h} = (h(x_1), h(x_2), \dots, h(x_N))^{\mathrm{T}},$$

and $\tilde{\boldsymbol{v}}_-$ is a vector of $\left\{\left(\left(\frac{2}{T}\right)^{\mu} b(x_j) - \lambda\right) Q_0^{\mu}(x_j)\right\}_{j=1}^{N}$.

For $\mu \in (1, 2)$, we look for

$$u_N(x) = g_0\, Q_0^{\mu}(x) + \frac{T}{2} g_1\, Q_{-1}^{\mu}(x) + \sum_{j=1}^{N} \tilde{v}_j\, Q_j^{\mu}(x), \tag{80}$$

and similarly, we can obtain

$$\left(\boldsymbol{I}_N + \left(\left(\frac{2}{T}\right)^{\mu} \boldsymbol{\Lambda}_b - \lambda\right)\boldsymbol{Q}_{\text{in}}^{\mu}\right) \tilde{\boldsymbol{v}} = \left(\frac{T}{2}\right)^{\mu} \boldsymbol{h} - g_0 \tilde{\boldsymbol{v}}_- - \frac{T}{2} g_1 \tilde{\boldsymbol{v}}_+, \tag{81}$$

and $\tilde{\boldsymbol{v}}_+$ is a vector of $\left\{\left((T/2)^{\mu} b(x_i) - \lambda\right) Q_{-1}^{\mu}(x_i)\right\}_{i=1}^{N}$.

Example 1 We take $a(t) = 1$ and $T = 2$ in (75). The initial conditions g_0, g_1 and $f(t)$ are given by

$$g_0 = 1, \quad g_1 = 1, \quad f(t) = \sin(t-1).$$

We use a bigger N (based on the criterion that even larger N does not lead to better accurate approximation) to produce to a reference "exact" solution, and measure the errors in L^{∞} -norm. Such a setting also applies to all examples below.

To show the convergence behaviour and accuracy, we plot in Fig. 3 the errors (in log-scale) for various N and different samples of μ. It is evident that the proposed method enjoys a spectral accuracy, and the errors decay exponentially. Indeed, the rapid convergence is observed for small N and all samples of μ.

For comparison, we depict in Fig. 4 the convergence behaviour of the polynomial-based collocation method in [27] in exactly the same setting. As expected, the polynomial approximation has a limited order of convergence for such a singular solution.

Example 2 We now consider (75) with a variable coefficient by taking $a(t) = 1 + \varepsilon\cos(t-1)$ and $T = 2$. The initial conditions g_0, g_1 and $f(t)$ are given by

$$g_0 = 1, \quad g_1 = 1, \quad f(t) = \sin(t-1).$$

It is known that the solution has a singular behaviour different from the constant coefficient case. The error plots in Fig. 5 illustrate that (i) there is a rapid convergence with a transition to a very slower rate; and (ii) the convergence rate varies with the magnitude of the perturbation parameter ε. However, the dependence is less for larger μ.

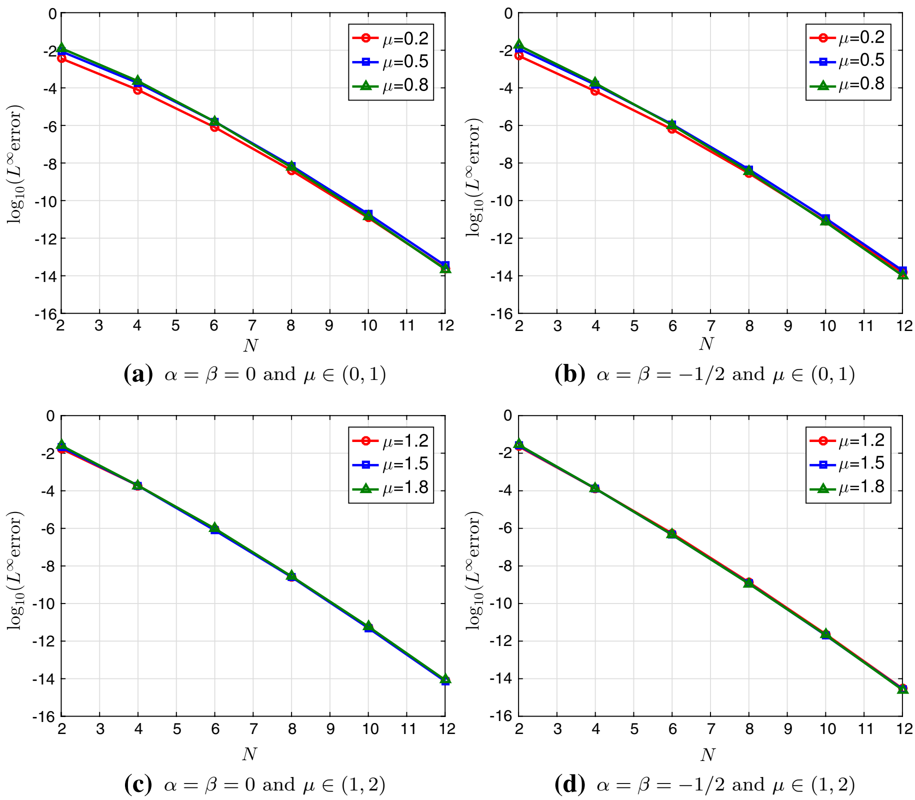
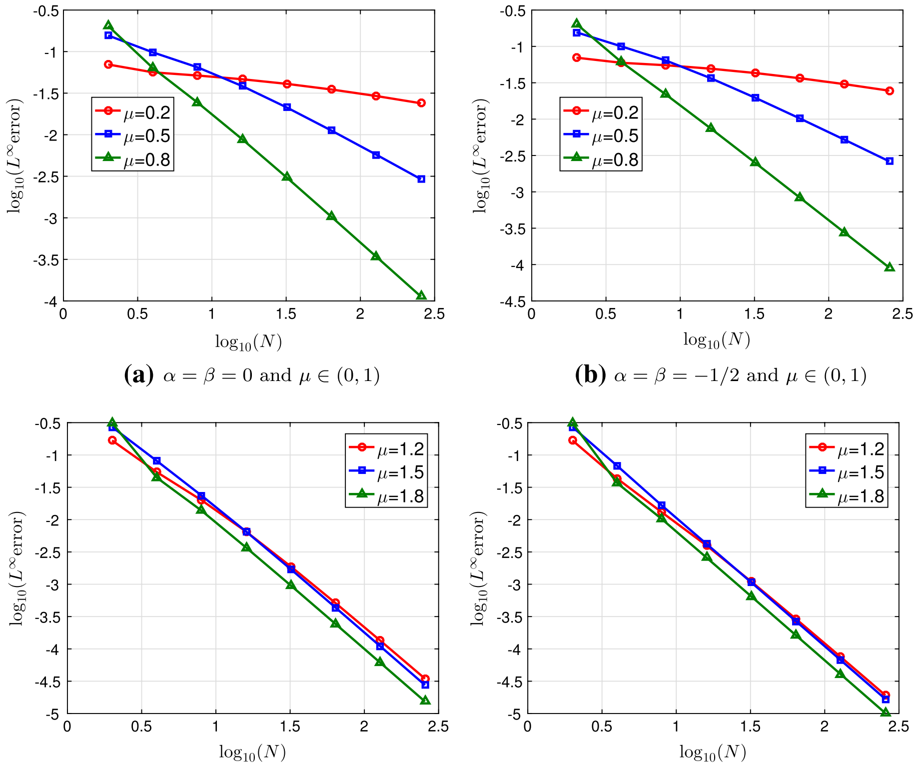


Fig. 3 $\log_{10}(L^\infty\text{-error})$ against N for Example 1 with $\lambda = 1$ and several μ



(a) $\alpha = \beta = 0$ and $\mu \in (0,1)$ **(b)** $\alpha = \beta = -1/2$ and $\mu \in (0,1)$

(c) $\alpha = \beta = 0$ and $\mu \in (1,2)$ **(d)** $\alpha = \beta = -1/2$ and $\mu \in (1,2)$

Fig. 4 Comparison with the polynomial-based collocation method in [27]: L^∞-error against N in log-log scale for Example 1 in the same setting as Fig. 3

5.2 Time-Fractional PDEs

Consider the time-fractional diffusion equation or wave equation

$$\begin{aligned} &{}_0^C D_t^\mu u(x,t) = a\,\partial_x^2 u(x,t) + f(x,t), \quad (x,t) \in (-1,1)\times(0,T], \\ &u(\pm 1, t) = 0, \quad t > 0, \end{aligned} \tag{82}$$

with initial condition(s)

$$u(x,0) = u_0(x), \quad x \in \Lambda, \quad \text{for} \quad \mu \in (0,1), \tag{83}$$

or

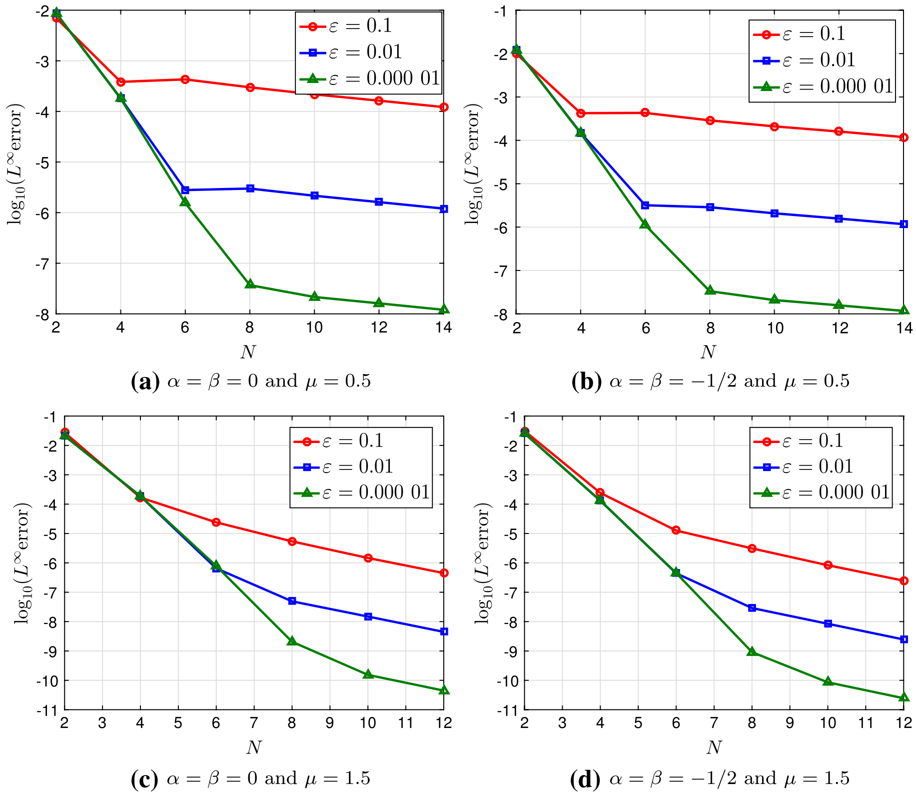
$$u(x,0) = u_0(x), \quad \partial_t u(x,0) = u_1(x), \quad x \in \Lambda, \quad \text{for} \quad \mu \in (1,2), \tag{84}$$

where f, u_0 and u_1 are given smooth functions.

We discretise the problem (82) using the Legendre-Galerkin method in space with the Fourier-like basis functions (cf. [42]). More precisely, the spatial Legendre-Galerkin approximation of (82) is to find $u_M(t) \in V_M := \{u \in \mathcal{P}_M : u(\pm 1) = 0\}$ such that

$$\big({}_0^C D_t^\mu u_M, v\big) + a(\partial_x u_M, \partial_x v) = (f, v), \quad \forall v \in V_M, \tag{85}$$

where $(u,v) := \int_{-1}^{1} uv\mathrm{d}x$ is the scalar product in $L^2(\Lambda)$.



(a) $\alpha = \beta = 0$ and $\mu = 0.5$ **(b)** $\alpha = \beta = -1/2$ and $\mu = 0.5$

(c) $\alpha = \beta = 0$ and $\mu = 1.5$ **(d)** $\alpha = \beta = -1/2$ and $\mu = 1.5$

Fig. 5 $\log_{10}(L^\infty$-error) against N with $\lambda = 1$ and various ε for Example 2

Lemma 5.1 (see [39, Lem. 2.1]) *Let us denote*

$$c_k = \frac{1}{\sqrt{4k+6}}, \quad \gamma_k(x) = c_k(P_k(x) - P_{k+2}(x)),$$
$$s_{jk} = \int_{-1}^{1} \gamma_k'(x)\gamma_j'(x)\mathrm{d}x, \quad m_{jk} = \int_{-1}^{1} \gamma_k(x)\gamma_j(x)\mathrm{d}x,$$

where $P_n(x)$ is the Legendre polynomial of degree n. Then we have

$$s_{jk} = \begin{cases} 1, & k = j, \\ 0, & k \neq j, \end{cases} \qquad m_{jk} = m_{kj} = \begin{cases} c_k c_j\left(\frac{2}{2j+1} + \frac{2}{2j+5}\right), & k = j, \\ -c_k c_j \frac{2}{2k+1}, & k = j+2, \\ 0, & \textit{otherwise}. \end{cases}$$

We expand $u_N(x,t)$ as

$$u_M(x,t)=\sum_{i=0}^{M-2}\widetilde{u}_i(t)\gamma_i(x). \tag{86}$$

Substituting $u_M(x,t)$ into (85) and taking $v=\gamma_j(x)$ for $0\le j\le M-2$, we obtain

$$({}_0^CD_t^{\mu}u_M,\gamma_j(x))+a(\partial_x u_M,\partial_x\gamma_j(x))=(f(x,t),\gamma_j(x)),\quad j=0,1,\dots,M-2. \tag{87}$$

Denote

$$\begin{aligned}&\boldsymbol{M}=(m_{kj})_{(M-1)\times(M-1)},\quad \widetilde{\boldsymbol{u}}_M(t)=[\widetilde{u}_0(t),\dots,\widetilde{u}_{M-2}(t)]^{\mathrm{T}},\\ &\widetilde{\boldsymbol{f}}(t)=\big[(f(x,t),\gamma_0(x)),\dots,(f(x,t),\gamma_{M-2}(x))\big]^{\mathrm{T}}.\end{aligned}$$

From Lemma 5.1, we find (87) is equivalent to the matrix equation:

$$\boldsymbol{M}\,{}_0^CD_t^{\mu}\widetilde{\boldsymbol{u}}_M+a\widetilde{\boldsymbol{u}}_M=\widetilde{\boldsymbol{f}}. \tag{88}$$

Note that the mass matrix $\boldsymbol{M}$ is a symmetric positive definite matrix, so its eigenvalues are all real and positive. Then there exists an orthogonal matrix $\boldsymbol{E}$ such that $\boldsymbol{E}^{\mathrm{T}}\boldsymbol{M}\boldsymbol{E}=\boldsymbol{D}$, where $\boldsymbol{D}=\mathrm{diag}(\lambda_0,\dots,\lambda_{M-2})$ with $\{\lambda_i>0\}_{i=0}^{M-2}$ being the eigenvalues of $\boldsymbol{M}$. Define

$$[\widehat{\gamma}_0(x),\dots,\widehat{\gamma}_{M-2}(x)]:=[\gamma_0(x),\dots,\gamma_{M-2}(x)]\boldsymbol{E}, \tag{89}$$

as a new basis of V_M satisfying

$$\begin{aligned}(\widehat{\gamma}_i(x),\widehat{\gamma}_j(x))&=\int_{-1}^{1}\boldsymbol{E}(:,i)^{\mathrm{T}}[\gamma_0(x),\dots,\gamma_{M-2}(x)]^{\mathrm{T}}[\gamma_0(x),\dots,\gamma_{M-2}(x)]\boldsymbol{E}(:,j)\mathrm{d}x\\ &=\boldsymbol{E}(:,i)^{\mathrm{T}}\boldsymbol{M}\boldsymbol{E}(:,j)=\boldsymbol{E}(:,i)^{\mathrm{T}}\big(\boldsymbol{E}\boldsymbol{D}\boldsymbol{E}^{\mathrm{T}}\big)\boldsymbol{E}(:,j)=\lambda_i\delta_{ij},\end{aligned} \tag{90}$$

and

$$\begin{aligned}(\widehat{\gamma}_i'(x),\widehat{\gamma}_j'(x))&=\int_{-1}^{1}\boldsymbol{E}(:,i)^{\mathrm{T}}[\gamma_0'(x),\dots,\gamma_{M-2}'(x)]^{\mathrm{T}}[\gamma_0'(x),\dots,\gamma_{M-2}'(x)]\boldsymbol{E}(:,j)\mathrm{d}x\\ &=\boldsymbol{E}(:,i)^{\mathrm{T}}\boldsymbol{I}_{M-1}\boldsymbol{E}(:,j)=\delta_{ij},\end{aligned} \tag{91}$$

where $\boldsymbol{I}_{M-1}$ is the identity matrix of order $M-1$.

Let us write

$$u_M(x,t)=\sum_{j=0}^{M-2}\widehat{u}_j(t)\widehat{\gamma}_j(x).$$

Taking $v=\widehat{\gamma}_l(x)$ in (85) and using (90) and (91), we find

$${}_0^CD_t^{\mu}\widehat{u}_l+a\lambda_l^{-1}\widehat{u}_l=\lambda_l^{-1}\widehat{f}_l(t),\quad l=0,\dots,M-2, \tag{92}$$

where $\widehat{f}_l(t)=(f(x,t),\widehat{\gamma}_l(x))$. For the initial data, we write

$$u_M(x,0)=\sum_{j=0}^{M-2}\widehat{u}_j(0)\widehat{\gamma}_j(x),\quad u_M'(x,0)=\sum_{j=0}^{M-2}\widehat{u}_j^1(0)\widehat{\gamma}_j(x),$$

where we determine the coefficients by

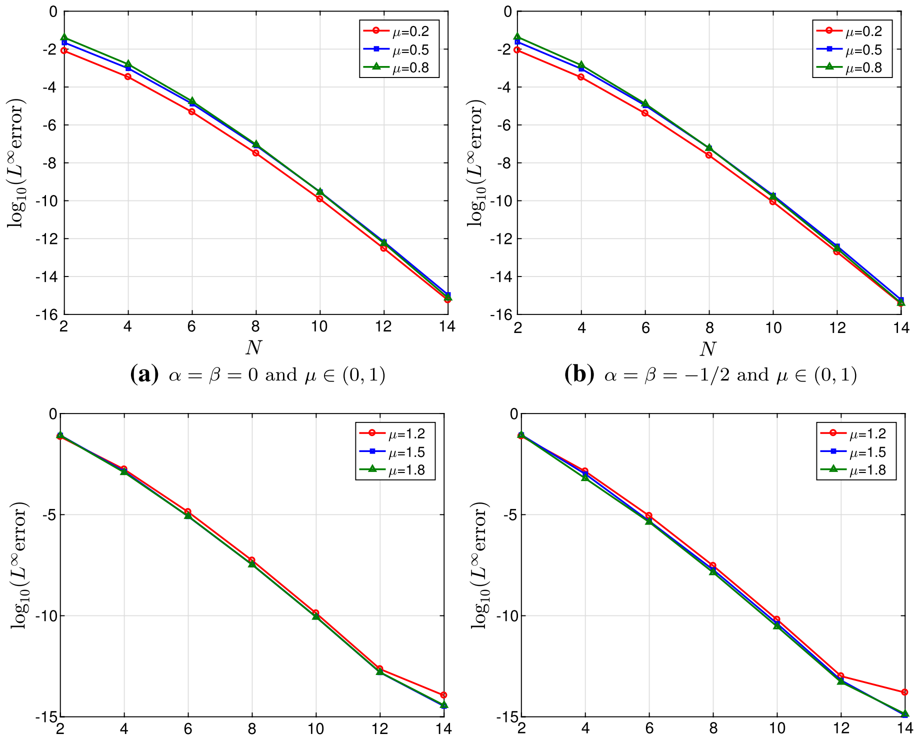
$$(u_M(\cdot,0)-u_0,\widehat{\gamma}_l)=0,\quad (u_M'(\cdot,0)-u_1,\widehat{\gamma}_l)=0,$$

for $0\le l\le M-2$. Then we can apply the collocation method described in Subsection 5.1 to solve (92) with the initial condition(s) for each mode.

Example 3 We consider problem (82) with $a=1$ and $T=2$. The initial conditions u_0, u_1, and $f(x,t)$ are given by

$$u_0=\sin(\pi x),\quad u_1=\cos(\pi x),\quad f(x,t)=\cos(x+t).$$

In Fig. 6, we plot the errors of the space-time spectral method, which indicates an exponential decay of the error for smooth inputs.



(a) $\alpha=\beta=0$ and $\mu\in(0,1)$ **(b)** $\alpha=\beta=-1/2$ and $\mu\in(0,1)$

(c) $\alpha=\beta=0$ and $\mu\in(1,2)$ **(d)** $\alpha=\beta=-1/2$ and $\mu\in(1,2)$

Fig. 6 $\log_{10}(L^\infty$-error) against N for Example 3

5.3 Concluding Remarks

In this paper, we introduced new non-polynomial basis functions for certain class of time-fractional PDEs. The construction of the new basis was based upon some generalised Birkhoff interpolation problem. Such a basis and the associated fractional collocation matrices could be computed in a fast recursive manner. With the singular basis tailored to some prototypical time-fractional PDEs, we could achieve very accurate approximation (with spectral accuracy at times) to some more general problems of similar nature.

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