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RESEARCH PAPER

NONSTANDARD GAUSS–LOBATTO QUADRATURE APPROXIMATION TO FRACTIONAL DERIVATIVES

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Dedicated to Professor Ivan Dimovski
on the occasion of his 80th anniversary

Abstract

A family of nonstandard Gauss-Jacobi-Lobatto quadratures for numerical calculating integrals of the form $\int_{-1}^{1} f'(x)(1-x)^\alpha \, dx$, $\alpha > -1$, is derived and applied to approximation of the usual fractional derivative. A software implementation of such quadratures was done by the recent MATHEMATICA package `OrthogonalPolynomials` (cf. [A.S. Cvetković, G.V. Milovanović, Facta Univ. Ser. Math. Inform. **19** (2004), 17–36] and [G.V. Milovanović, A.S. Cvetković, Math. Balkanica **26** (2012), 169–184]). Several numerical examples are presented and they show the effectiveness of the proposed approach.

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1. Introduction

Fractional calculus (including the operators of fractional order integration and differentiation) has been often used in modelling many physical and engineering problems. We refer the reader to [2, 3, 21, 22, 25, 36, 38] for

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a general theory, as well as a description of the main applications in fields ranging from mechanics, biology to biomechanics, diagnostic imaging, electrochemistry, finance, sustainable environment and renewable energy. A theory of the generalized fractional calculus, as well as the corresponding applications, can be found in a monograph written by Kiryakova [23]. We also mention a few the most cited papers on this subject [17, 26, 27, 5].

The fractional derivative $D_*^q f(t)$ in the Caputo version [6] and the Riemann–Liouville fractional derivative ${}_0D_t^q f(t)$, where $0 < q < 1$, are defined by

$$D_*^q f(t) = \frac{1}{\Gamma(1-q)} \int_0^t f'(s)(t-s)^{-q}\,\mathrm{d}s, \quad t > 0, \tag{1.1}$$

$${}_0D_t^q f(t) = \frac{1}{\Gamma(1-q)} \frac{\mathrm{d}}{\mathrm{d}t} \int_0^t f(s)(t-s)^{-q}\,\mathrm{d}s, \quad t > 0, \tag{1.2}$$

respectively [36]. It is well-known that the fractional derivative of Riemann–Liouville and Caputo type are closely linked by the following relationship:

$${}_0D_t^q f(t) = \frac{f(0)}{t^q\Gamma(1-q)} + D_*^q f(t). \tag{1.3}$$

The operator of fractional derivative is more complicated than the classical one, and its calculation is also more difficult than in the integer order case.

In this paper we construct a quadrature method for approximating the fractional derivative defined by (1.1) or (1.2). Although there is comprehensive literature on the numerical methods for solving equations involving fractional derivatives and integrals (cf. [8, 9, 11, 3, 10, 35]), there seems to exist a few literature on automatic quadrature for the fractional derivatives, see e.g. [20, 24, 39].

Let $w(x)$ be a nonnegative weight function on the interval (a, b) that vanishes only at isolated points. We consider an n-point quadrature formula

$$\int_a^b f(x)w(x)\,\mathrm{d}x = \sum_{k=1}^{n} A_k f(x_k) + R_n[f], \tag{1.4}$$

where the sum $Q_n[f] = \sum_{k=1}^n A_k f(x_k)$ provides an approximation to the integral $\int_a^b f(x)w(x)\,\mathrm{d}x$ and $R_n[f]$ is the corresponding error. We shall always require $a \le x_1 < x_2 < \cdots < x_n \le b$. In the quadrature sum $Q_n[f]$, the points x_k are called the nodes and A_k are the weights of the quadrature formula (1.4). The mentioned quadrature rules use the information on the integrand only at some selected points x_k, $k = 1, \ldots, n$ (the values of the function f). Such quadratures will be called the standard quadrature formulae, see [4, 28, 40].

The quadrature formula (1.4) with the maximal algebraic degree of exactness $2n-1$ is called the Gaussian quadrature formula. Indeed, if $\mathbb{P}_d$ be the set of all algebraic polynomials of degree at most d then in the Gaussian quadrature formula (1.4) we have $R_n[p]=0$ for all $p\in\mathbb{P}_{2n-1}$.

This paper is organized as follows. In Section **2** we give a short account on Gauss-Jacobi quadrature rules and the corresponding Lobatto modification. Some remarks on nonstandard Gaussian quadratures are mentioned in Section **4**. Main result on the Gauss-Jacobi-Lobatto nonstandard quadrature is proved in Section **4**, as well as the corresponding software implementation in MATHEMATICA. Finally, applications to an approximation of fractional derivatives and numerical examples are presented in Sections **5** and **6**, respectively. Several numerical examples show the effectiveness of the proposed approach.

2. Gauss–Jacobi quadrature rules and the Lobatto modification

Let $w^{\alpha,\beta}(x):=(1-x)^\alpha(1+x)^\beta$ with parameters $\alpha,\beta>-1$ be the Jacobi weight function on the interval $(-1,1)$. The Jacobi polynomials, denoted by $P_n^{(\alpha,\beta)}(x)$, are mutually orthogonal on the interval $(-1,1)$ with respect to the $w^{\alpha,\beta}(x)$. This means that

$$\int_{-1}^{1} P_n^{(\alpha,\beta)}(x)P_m^{(\alpha,\beta)}(x)w^{\alpha,\beta}(x)\,\mathrm{d}x=0 \quad n\neq m. \tag{2.1}$$

An n-point quadrature rule for the weight function $w^{\alpha,\beta}$ is called a formula of the type

$$\int_{-1}^{1} f(x)w^{\alpha,\beta}(x)\,\mathrm{d}x=\sum_{k=1}^{n} w_k^{\alpha,\beta} f(x_k^{\alpha,\beta})+R_n[f]. \tag{2.2}$$

A quadrature rule (2.2) with degree of exactness $n-1$ is called interpolatory. These are precisely those obtained by interpolation, that is, for which

$$w_j^{\alpha,\beta}=\int_{-1}^{1}\ell_j(x)w^{\alpha,\beta}(x)\,\mathrm{d}x, \quad j=1,\dots,n, \tag{2.3}$$

where $\ell_j\in\mathbb{P}_{n-1}$ are the Lagrange polynomials associated with the nodes $x_k^{\alpha,\beta}$ such that $\ell_j(x_k^{\alpha,\beta})=\delta_{jk}$, for $j,k=1,\dots,n$.

We now discuss the relation between the Jacobi polynomials and the Gauss–type quadratures. The mechanism of a Gauss–type quadrature is to seek the best numerical approximation of an integral by selecting optimal nodes at which integrand is evaluated. It can be proved that the nodes $x_k^{\alpha,\beta}$ in a Gauss–Jacobi quadrature are the roots of the Jacobi polynomial $P_n^{(\alpha,\beta)}$, that is

$$P_n^{(\alpha,\beta)}(x_k^{\alpha,\beta})=0, \quad k=1,\dots,n. \tag{2.4}$$

All nodes $x_k^{\alpha,\beta}$ are real, distinct, and contained in the open interval $(-1,1)$. The weights $w_k^{\alpha,\beta}$ are known in closed form as

$$w_k^{\alpha,\beta} = \frac{2^{\alpha+\beta+1}}{n!\Gamma(n+\alpha+\beta+1)} \cdot \frac{\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}{\Big(1-\big(x_k^{\alpha,\beta}\big)^2\Big)\left[\dfrac{\mathrm{d}}{\mathrm{d}x}P_n^{(\alpha,\beta)}\big(x_k^{\alpha,\beta}\big)\right]^2}, \qquad (2.5)$$

where $k=1,\dots,n$ (see, for instance, [28, p. 325]). We can thus conclude that the quadrature formula (2.2) with the nodes $x_k^{\alpha,\beta}$ prescribed by (2.4) and the weights $w_k^{\alpha,\beta}$ given by (2.3), has degree of exactness $2n-1$, the maximum value that can be achieved using interpolatory quadrature formulae with n nodes. This optimal formula is called the (standard) Gauss–Jacobi quadrature formula.

As n increases, finding roots of $P_n^{(\alpha,\beta)}$ become an ill-conditioned and time consuming problem. An alternative and today standard approach for finding the nodes and the weights of a Gaussian quadrature rule is to use the Golub-Welsch algorithm [15, 14].

Let $k_n^{\alpha,\beta}$ be the leading coefficient of $P_n^{(\alpha,\beta)}(x)$, i.e.,

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

It is well known that there exists a unique sequence of monic orthogonal polynomials $\pi_n^{\alpha,\beta}(x) = P_n^{(\alpha,\beta)}(x)/k_n^{\alpha,\beta}$. They can be generated by the three term recurrence relation [14, 28]

$$\pi_{k+1}^{\alpha,\beta}(x) = (x-\alpha_k^J)\pi_k^{\alpha,\beta}(x) - \beta_k^J\pi_{k-1}^{\alpha,\beta}(x), \quad k \ge 0, \qquad (2.6)$$

with starting values $\pi_{-1}^{\alpha,\beta}=0$, $\pi_0^{\alpha,\beta}=1$, and with the recursion coefficients

$$\alpha_k^J = \frac{\beta^2-\alpha^2}{(2k+\alpha+\beta)(2k+\alpha+\beta+2)}, \quad k \ge 0,$$

$$\beta_k^J = \frac{4k(k+\alpha)(k+\beta)(k+\alpha+\beta)}{(2k+\alpha+\beta)^2((2k+\alpha+\beta)^2-1)}, \quad k \ge 1.$$

This approach is based on determining the eigenvalues and normalized eigenvectors of the symmetric tridiagonal *Jacobi matrix*

$$\mathbf{J}_n = \mathrm{tridiag}\big(\boldsymbol{\beta}^J, \boldsymbol{\alpha}^J, \boldsymbol{\beta}^J\big) \in \mathbb{R}^{n\times n}, \qquad (2.7)$$

where

$$\boldsymbol{\alpha}^J = (\alpha_0^J, \alpha_1^J, \dots, \alpha_{n-1}^J)^T \in \mathbb{R}^n, \quad \boldsymbol{\beta}^J = \left(\sqrt{\beta_1^J}, \dots, \sqrt{\beta_{n-1}^J}\right)^T \in \mathbb{R}^{n-1}.$$

The elements of this matrix are obtained from the coefficients of the three-term recurrence relation (2.6). The nodes $x_k^{\alpha,\beta}$ in (2.2) are the eigenvalues of the matrix $\mathbf{J}_n$ and the corresponding weights $w_k^{\alpha,\beta}$ may be obtained from the first components of the normalized eigenvectors. For more details we refer the reader to [14, 15, 28]. An efficient algorithm for computation of Gauss–Jacobi quadrature nodes and weights for any $n \geq 100$ has been recently presented in [18].

The $(n+2)$–points Gauss–Lobatto quadrature rule for the Jacobi weight function is an interpolatory quadrature rule of the following form

$$\int_{-1}^{1} f(x)w^{\alpha,\beta}(x)\,\mathrm{d}x = \lambda_0^{\alpha,\beta} f(-1) + \sum_{k=1}^{n} \lambda_k^{\alpha,\beta} f(\zeta_k^{\alpha,\beta}) + \lambda_{n+1}^{\alpha,\beta} f(1) + R_n^{\alpha,\beta}[f], \tag{2.8}$$

with the maximal algebraic degree of exactness. The internal nodes $\zeta_k^{\alpha,\beta}$ are the zeros of the orthogonal polynomial of degree n with respect to the weight function $x \mapsto (1-x^2)w^{\alpha,\beta}(x)$ (cf. [28, pp. 330–332]). In this case, the Gauss–Lobatto points $\zeta_k^{\alpha,\beta}$ are the zeros of the polynomial $\dfrac{\mathrm{d}}{\mathrm{d}x} P_{n+1}^{(\alpha,\beta)}(x)$. It is well known that the Gauss–Lobatto quadrature (2.8) has degree of exactness $2n+1$, see [14, 28].

3. Nonstandard quadratures of Gaussian type

In many cases it is not possible to measure the exact value of the function f at points x_k, so that a standard quadrature cannot be applied. Thus, if the information data $\{f(x_k)\}_{k=1}^{n}$ in the standard quadrature (1.4) is replaced by $\{\mathscr{A}^{h_k} f(x_k)\}_{k=1}^{n}$, where $\mathscr{A}^h$ is an extension of some linear operator $\mathscr{A}^h : \mathbb{P} \to \mathbb{P}, h \geq 0$, where $\mathbb{P}$ is the set of all algebraic polynomials, we get a non-standard quadrature formula [33]

$$\int_a^b f(x)w(x)\,\mathrm{d}x = \sum_{k=1}^{n} w_k (\mathscr{A}^{h_k} f)(x_k) + R_m[f], \tag{3.1}$$

where w is a positive weight function on $[a,b]$.

In the sequel, we consider a non-standard m-point ($m > 2$) interpolatory quadrature of Gaussian type (precisely, of the Gauss-Lobatto type),

$$\int_a^b g'(x)w(x)\,\mathrm{d}x = \sum_{k=1}^{m} w_k g(x_k) + R_m[g], \tag{3.2}$$

which is exact on the set $\mathbb{P}_{2m-3}$, i.e., $R_m(\mathbb{P}_{2m-3}) = 0$. If we put $g(x) = \int_c^x f(t)\,\mathrm{d}t$, where c is some constant, formula (3.2) reduces to

$$\int_a^b f(x)w(x)\,\mathrm{d}x = \sum_{k=1}^{m} w_k \int_c^{x_k} f(t)\,\mathrm{d}t + R_m[f],$$

which is a special case of the generalized nonstandard (operator) formulae (3.2) of Gaussian type.

Theorem **3.1**. *Given an integer k with $0 \le k \le m$, the quadrature formula* (3.2) *has degree of exactness $d = m - 1 + k$ if and only if both the following conditions are satisfied:*

(a) *Formula* (3.2) *is interpolatory.*

(b) *The node polynomial $\ell(x) := \prod_{\nu=1}^{m}(x - x_\nu)$ satisfies*

$$\int_a^b \big(\ell(x)p(x)\big)' w(x)\,\mathrm{d}x = 0, \tag{3.3}$$

for all $p \in \mathbb{P}_{k-1}$.

P r o o f. To prove this, we will follow a manner similar to that used in [14]. We first prove the necessity of (a) and (b). Since, by assumption, the degree of exactness is $d = m - 1 + k \ge m - 1$, condition (a) is trivial. condition (b) also follows immediately, since, for any $p \in \mathbb{P}_{k-1}$, the product $\ell(x)p(x)$ is in $\mathbb{P}_{m-1+k}$; hence,

$$\int_a^b \big(\ell(x)p(x)\big)' w(x)\,\mathrm{d}x = \sum_{\nu=1}^{m} w_\nu \ell(x_\nu)p(x_\nu) = 0.$$

To prove the sufficiency of (a) and (b), we must show that for any $p \in \mathbb{P}_{m-1+k}$ we have $R_m[p] = 0$ in (3.2). Given any such p, divide it by ℓ, so that

$$p(x) = q(x)\ell(x) + r(x), \quad q \in \mathbb{P}_{k-1}, \quad r \in \mathbb{P}_{m-1},$$

where $q(x)$ is the quotient and $r(x)$ is the corresponding remainder. There follows

$$\int_a^b p'(x)w(x)\,\mathrm{d}x = \int_a^b \big(\ell(x)q(x)\big)' w(x)\,\mathrm{d}x + \int_a^b r'(x)w(x)\,\mathrm{d}x$$

The first integral on the right vanishes by (b), since $q \in \mathbb{P}_{k-1}$, whereas the second, by (a), since $r \in \mathbb{P}_{m-1}$, equals

$$\sum_{\nu=1}^{m} w_\nu r(x_\nu)$$

by virtue of (a). But

$$r(x_\nu) = p(x_\nu) - q(x_\nu)\ell(x_\nu) = p(x_\nu),$$

so that indeed

$$\int_a^b p'(x)w(x)dx = \sum_{\nu=1}^{m} w_\nu p(x_\nu)$$

that is, $R_n[p] = 0$. This completes the proof. □

4. Gauss-Jacobi-Lobatto nonstandard quadratures

As an interesting special case for application to fractional derivatives, we consider the nonstandard Gauss–Lobatto quadrature rule, with respect to a special Jacobi weight $w^{\alpha,0}(x) = (1-x)^\alpha$, $\alpha > -1$,

$$\int_{-1}^{1} g'(x)w^{\alpha,0}(x)\,\mathrm{d}x = \lambda_0^{\alpha,0} g(-1) + \sum_{k=1}^{n} \lambda_k^{\alpha,0} g(\xi_k^{\alpha,1}) + \lambda_{n+1}^{\alpha,0} g(1) + R_n^{\alpha,0}[g]. \tag{4.1}$$

Our main result can be stated in the following form:

THEOREM **4.1**. *Let $-1 = \xi_0^{\alpha,1} < \xi_1^{\alpha,1} < \cdots < \xi_n^{\alpha,1} < \xi_{n+1}^{\alpha,1} = 1$ be the zeros of the polynomial $(1-x^2)P_n^{(\alpha,1)}(x)$, and let the weights $\lambda_k^{\alpha,0}$ be as*

$$\lambda_k^{\alpha,0} = \frac{\alpha w_k^{\alpha,1}}{1-(\xi_k^{\alpha,1})^2}, \quad k = 1,\ldots,n, \tag{4.2}$$

and

$$\lambda_0^{\alpha,0} = -2^\alpha \frac{n^2+(\alpha+2)n+1}{(n+1)(n+\alpha+1)}, \quad \lambda_{n+1}^{\alpha,0} = -\lambda_0^{\alpha,0} - \sum_{k=1}^{n} \lambda_k^{\alpha,0}, \tag{4.3}$$

where $w_k^{\alpha,1}$, $k = 1,\ldots,n$, are the Christoffel numbers in the standard Gauss-Jacobi quadrature with respect to the weight function $w^{\alpha,1}(x) = (1-x)^\alpha(1+x)$, $\alpha > -1$, which correspond to the nodes $\xi_k^{\alpha,1}$, $k = 1,\ldots,n$.

Then the quadrature formula (4.1) *has the maximal degree of precision, i.e., it is exact for each polynomial of degree at most $2n+1$.*

P r o o f. Suppose that $\omega(x) = (1-x^2)P_n^{(\alpha,1)}(x)$ and

$$\lambda_k^{\alpha,0} = \int_{-1}^{1} \ell_k'(x)w^{\alpha,0}(x)\,\mathrm{d}x, \quad k = 0,1,\ldots,n+1, \tag{4.4}$$

where $\ell_k \in \mathbb{P}_{n+1}$ are the Lagrange polynomials associated with the nodes $\xi_k^{\alpha,1}$. It is obvious that the quadrature (4.1) with these weights (4.4) is at least interpolatory. According to Theorem **3.1**, it is enough to show the orthogonality relation (3.3) for each $p \in \mathbb{P}_{n-1}$. To do this, we apply integration by parts to obtain

$$\int_{-1}^{1} \big(\omega(x)p(x)\big)' w^{\alpha,0}(x)\,\mathrm{d}x = \alpha \int_{-1}^{1} P_n^{(\alpha,1)}(x)p(x)w^{\alpha,1}(x)\,\mathrm{d}x = \alpha\langle P_n^{(\alpha,1)}, p\rangle.$$

Then, because of orthogonality of $P_n^{(\alpha,1)}$ to $\mathbb{P}_{n-1}$ with respect to $w^{\alpha,1}$ on $(-1,1)$, we conclude that

$$(\forall p\in\mathbb{P}_{n-1})\qquad \int_{-1}^{1}\big(\omega(x)p(x)\big)'w^{\alpha,0}(x)\,\mathrm{d}x=\alpha\langle P_n^{(\alpha,1)},p\rangle=0.$$

Now, we denote the "node" polynomial by $\ell(x)=(x^2-1)\pi_n(x)$, where $\pi_n\equiv\pi_n^{\alpha,1}$ is the monic Jacobi polynomial with parameters α and $\beta=1$.

In order to compute the weights $\lambda_k^{\alpha,0}$, corresponding to the set of nodes $\xi_k^{\alpha,1}$, we use the formulas (4.4).

Since $\ell'(x)=2x\pi_n(x)+(x^2-1)\pi_n'(x)$, for the endpoints ±1, we have

$$\ell'(\xi_0^{\alpha,1})=\ell'(-1)=-2\pi_n(-1),\quad \ell'(\xi_{n+1}^{\alpha,1})=\ell'(1)=2\pi_n(1).$$

At the zeros of the Jacobi polynomial π_n, we have

$$\ell'(\xi_k^{\alpha,1})=\big((\xi_k^{\alpha,1})^2-1\big)\pi_n'(\xi_k^{\alpha,1}),\quad k=1,\ldots,n.$$

The corresponding Lagrange polynomials associated with the nodes $\xi_k^{\alpha,1}$,

$$\ell_k(x)=\frac{\ell(x)}{\ell'(\xi_k^{\alpha,1})\big(x-\xi_k^{\alpha,1}\big)},\quad k=0,1,\ldots,n+1, \tag{4.5}$$

can be expressed in the following form

$$\ell_0(x)=\frac{(1-x)\pi_n(x)}{2\pi_n(-1)},\quad \ell_{n+1}(x)=\frac{(1+x)\pi_n(x)}{2\pi_n(1)}$$

and

$$\ell_k(x)=\frac{1-x^2}{1-\big(\xi_k^{\alpha,1}\big)^2}\cdot\frac{\pi_n(x)}{\pi_n'(\xi_k^{\alpha,1})\big(x-\xi_k^{\alpha,1}\big)},\quad k=1,\ldots,n.$$

Now we need derivatives of the Lagrange polynomials, i.e.,

$$\ell_0'(x)=\frac{(1-x)\pi_n'(x)-\pi_n(x)}{2\pi_n(-1)},\quad \ell_{n+1}'(x)=\frac{(1+x)\pi_n'(x)+\pi_n(x)}{2\pi_n(1)}$$

and

$$\ell_k'(x)=\frac{1}{1-\big(\xi_k^{\alpha,1}\big)^2}\left\{-2x\,\ell_k^G(x)+(1-x^2)\frac{\mathrm{d}}{\mathrm{d}x}\left[\ell_k^G(x)\right]\right\},\quad k=1,\ldots,n,$$

where $\ell_k^G(x)$, $k=1,\ldots,n$, are Lagrange polynomials associated with the nodes $\xi_k^{\alpha,1}$ for which

$$\int_{-1}^{1}\ell_k^G(x)w^{\alpha,1}(x)\,\mathrm{d}x=w_k^{\alpha,1},\quad k=1,\ldots,n,$$

where $w_k^{\alpha,1}$ are the Christoffel numbers in the corresponding Gauss-Jacobi quadrature rule with respect to the weight $w^{\alpha,1}$ on $(-1,1)$.

Thus, for $k=1,\ldots,n$, we get

$$\begin{aligned}
\lambda_k^{\alpha,0} &= \int_{-1}^{1} \ell_k'(x) w^{\alpha,0}(x)\,\mathrm{d}x \\
&= \frac{1}{1-\left(\xi_k^{\alpha,1}\right)^2}\left\{\int_{-1}^{1}[(1-x)-(1+x)]\ell_k^G(x) w^{\alpha,0}(x)\,\mathrm{d}x \right. \\
&\qquad \left. + \int_{-1}^{1}(1-x^2)\frac{\mathrm{d}}{\mathrm{d}x}\left[\ell_k^G(x)\right] w^{\alpha,0}(x)\,\mathrm{d}x\right\} \\
&= \frac{1}{1-\left(\xi_k^{\alpha,1}\right)^2}\left\{\int_{-1}^{1}\ell_k^G(x) w^{\alpha+1,0}(x)\,\mathrm{d}x - \int_{-1}^{1}\ell_k^G(x) w^{\alpha,1}(x)\,\mathrm{d}x \right. \\
&\qquad \left. + \int_{-1}^{1}\frac{\mathrm{d}}{\mathrm{d}x}\left[\ell_k^G(x)\right] w^{\alpha+1,1}(x)\,\mathrm{d}x\right\}.
\end{aligned}$$

Using integration by parts, the last integral becomes

$$\begin{aligned}
\int_{-1}^{1}\frac{\mathrm{d}}{\mathrm{d}x}\left[\ell_k^G(x)\right] w^{\alpha+1,1}(x)\,\mathrm{d}x &= (\alpha+1)\int_{-1}^{1}\ell_k^G(x) w^{\alpha,1}(x)\,\mathrm{d}x \\
&\quad - \int_{-1}^{1}\ell_k^G(x) w^{\alpha+1,0}(x)\,\mathrm{d}x,
\end{aligned}$$

so that we get

$$\lambda_k^{\alpha,0} = \frac{\alpha}{1-(\xi_k^{\alpha,1})^2}\int_{-1}^{1}\ell_k^G(x) w^{\alpha,1}(x)\,\mathrm{d}x = \frac{\alpha w_k^{\alpha,1}}{1-(\xi_k^{\alpha,1})^2}, \quad k=1,\ldots,n,$$

i.e., (4.2).

For $k=0$ we have

$$\begin{aligned}
\lambda_0^{\alpha,0} &= \int_{-1}^{1}\ell_0'(x) w^{\alpha,0}(x)\,\mathrm{d}x \\
&= \frac{1}{2\pi_n(-1)}\int_{-1}^{1}\big[(1-x)\pi_n'(x)-\pi_n(x)\big] w^{\alpha,0}(x)\,\mathrm{d}x \\
&= \frac{1}{2\pi_n(-1)}\left\{\int_{-1}^{1}\pi_n'(x) w^{\alpha+1,0}(x)\,\mathrm{d}x - \int_{-1}^{1}\pi_n(x) w^{\alpha,0}(x)\,\mathrm{d}x\right\}.
\end{aligned}$$

Since

$$\int_{-1}^{1}\pi_n'(x) w^{\alpha+1,0}(x)\,\mathrm{d}x = -\pi_n(-1)2^{\alpha+1} + (\alpha+1)\int_{-1}^{1}\pi_n(x) w^{\alpha,0}(x)\,\mathrm{d}x,$$

we get

$$\lambda_0^{\alpha,0} = \frac{1}{2\pi_n(-1)} \left\{ \alpha \int_{-1}^{1} \pi_n(x) w^{\alpha,0}(x)\,\mathrm{d}x - 2^{\alpha+1}\pi_n(-1) \right\}.$$

If we introduce the so-called function of the second kind (cf. [28, p. 117])

$$f_n(z) = \int_{-1}^{1} \frac{\pi_n(x)}{z-x}\, w^{\alpha,1}(x)\,\mathrm{d}x$$

we see that for $z=-1$, it reduces to

$$f_n(-1) = -\int_{-1}^{1} \frac{\pi_n(x)}{1+x}\, w^{\alpha,1}(x)\,\mathrm{d}x = -\int_{-1}^{1} \pi_n(x) w^{\alpha,0}(x)\,\mathrm{d}x,$$

so that

$$\lambda_0^{\alpha,0} = -\frac{\alpha}{2}\cdot\frac{f_n(-1)}{\pi_n(-1)} - 2^{\alpha}. \tag{4.6}$$

In order to determine $f_n(-1)$ we start with the following equality for Jacobi polynomials (cf. [1, p. 304])

$$(2n+\alpha+1)P_n^{(\alpha,0)}(x) = (n+\alpha+1)P_n^{(\alpha,1)}(x) + (n+\alpha)P_{n-1}^{(\alpha,1)}(x).$$

Transforming it to monic polynomials, multiplying by $w^{\alpha,0}(x)$, and integrating it over $(-1,1)$, we obtain the folloing relation

$$(2n+\alpha+1)f_n(-1) + \frac{2n(n+\alpha)}{2n+\alpha} f_{n-1}(-1) = -\frac{2n+\alpha+1}{\alpha+1} 2^{\alpha+1}\delta_{n,0}, \tag{4.7}$$

where $\delta_{i,j}$ is Kronecker's delta. This gives

$$f_0(-1) = -\frac{2^{\alpha+1}}{\alpha+1}, \quad f_n(-1) = -\frac{2n(n+\alpha)}{(2n+\alpha)(2n+\alpha+1)} f_{n-1}(-1), \quad n \ge 1,$$

i.e.,

$$f_n(-1) = (-1)^{n+1} \frac{2^{n+\alpha+1} n!}{(n+\alpha+1)_{n+1}}, \quad n = 0,1,2,\ldots\ .$$

Since $\pi_n(-1) = \pi_n^{\alpha,1}(-1) = (-1)^n 2^n (n+1)!/(n+\alpha+2)_n$, from (4.6) we find $\lambda_0^{\alpha,0}$ in the form given in (4.3).

Finally, because of $\sum_{k=0}^{n+1} \lambda_k^{\alpha,0} = 0$, we obtain the second formula in (4.3). □

Remark **4.1**. The weights at the endpoints can be also expressed in the form

$$\lambda_0^{\alpha,0} = -\frac{2^{\alpha}}{\alpha+1} - \frac{\alpha}{2}\sum_{k=1}^{n} \frac{w_k^{\alpha,1}}{1+\xi_k^{\alpha,1}}, \quad \lambda_{n+1}^{\alpha,0} = \frac{2^{\alpha}}{\alpha+1} - \frac{\alpha}{2}\sum_{k=1}^{n} \frac{w_k^{\alpha,1}}{1-\xi_k^{\alpha,1}}.$$

Thus, there are simple explicit formulae for the weights $\lambda_j^{\alpha,0}$, $j = 0, 1, \ldots, n+1$. An alternative way for finding these coefficients are considered in [12].

4.1. Software implementation

The construction of the Gauss-Jacobi-Lobatto nonstandard quadrature (4.1) for an arbitrary $n \in \mathbb{N}$ and each $\alpha > -1$ can be realized very easy by our MATHEMATICA package `OrthogonalPolynomials` (see [7] and [34]). Alternatively, for this purpose there is also Gautschi's package `SOPQ` written in MATLAB (cf. [31]). These packages provide many other calculations with orthogonal polynomials and different quadrature rules, and they are downloadable from Web Sites: `http://www.mi.sanu.ac.rs/~gvm/` and `http://www.cs.purdue.edu/archives/2002/wxg/codes/`, respecively.

The corresponding MATHEMATICA code for constructing parameters of the quadrature formula (4.1) is:

```
<< orthogonalPolynomials`
LobattoParam[n_,alpha_,digits_]:=Module[{node,lambda,weight,k,a0,an1},
  {node,weight} = aGaussianNodesWeights[n,{aJacobi,alpha,1},
            WorkingPrecision -> digits+5, Precision->digits];
  a0 = 2^alpha(alpha/((n+1)(n+alpha+1))-1);
  lambda = alpha*weight/(1-node^2);
  an1 = -(a0+Sum[lambda[[k]],{k,1,n}]);
  lambda=N[Append[Prepend[lambda,a0],an1],digits];
  node=N[Append[Prepend[node,-1],1],digits]; Return[{node,lambda}]];
```

Variable–precision arithmetic enables us to calculate parameters (nodes and weights) in (4.1), named as `node` and `lambda`, i.e.,

$$\texttt{node} = (\xi_0^{\alpha,1}, \xi_1^{\alpha,1}, \ldots, \xi_{n+1}^{\alpha,1}) \quad \text{and} \quad \texttt{lambda} = (\lambda_0^{\alpha,0}, \lambda_1^{\alpha,0}, \ldots, \lambda_{n+1}^{\alpha,0}),$$

with an arbiytrary precision. The input parameter `digits` defines the so-called *working precision* in the form `WorkingPrecision -> digits+5`.

For example, taking `digits-> 20` for $\alpha = -1/2$ and $n = 5$ we get the following results:

```
In[1]:= {node, lambda} = LobattoParam[5, -1/2, 20]

Out[1]= {{-1.0000000000000000000, -0.78566926929466497066,
          -0.34243721374692749946, 0.19893554984718572955,
           0.68075005442268573279, 0.96270659305743529348,
           1.0000000000000000000},
         {-0.71782052029543460810, -0.072612263768525365535,
          -0.16642116952156041977, -0.37516617602834936907,
          -1.1131007878331247823,  -10.292032937247316885,
          12.737153854694311430}}
```

The corresponding MATLAB code for constructing parameters of the quadrature formula (4.1) is:

```
function [node,lambda]=LobattoParam(n,q)
ab=r_jacobi(n,-q,1); xw=gauss(n,ab);
node=xw(:,1); omega=xw(:,2);
lambda(1)= -2^(-q)*(q/((n+1)*(n-q+1))+1);
lambda(2:n+1)=-q*omega(1:n)./(1-node(1:n).^2);
lambda(n+2)= -sum(lambda(1:n+1));
node=[-1 node' 1];
```

5. Applications to an approximation of fractional derivatives

Let $f(s)$ be a sufficiently well-behaved function in $[-1,1]$. If $f(s)$ is defined in $[0,t]$ instead of $[-1,1]$, then change of variable $s=\frac{t}{2}(1+x)$ could transform $f(s)$ into $g(x):=f(\frac{t}{2}(1+x))$, where $x\in[-1,1]$. Rewrite the definition (1.1) in the equivalent form

$$D_*^q f(t)=\frac{2^q}{t^q\Gamma(1-q)}\int_{-1}^{1} g'(x)(1-x)^{-q}\,\mathrm{d}x. \tag{5.1}$$

To approximate the integral in (5.1), we use the nonstandard quadrature (4.1) with $\alpha:=-q$, i.e.,

$$(\forall g\in\mathbb{P}_{2n+1})\quad \int_{-1}^{1} g'(x)w^{-q,0}(x)\,\mathrm{d}x=\sum_{k=0}^{n+1}\lambda_k^{-q,0}g(\xi_k^{-q,1}), \tag{5.2}$$

where $\xi_k^{-q,1}$ are the zeros of the polynomial $(1-x^2)P_n^{(-q,1)}(x)$, and the weights $\lambda_j^{-q,0}$ are given by (4.2) and (4.3), in which $\alpha:=-q$. Thanks to the representation (5.1), the following approximation of the Caputo fractional derivative (1.1)

$$D_\star^q f(t)\approx D_{\star,n}^q f(t):=\frac{2^q}{t^q\Gamma(1-q)}\sum_{k=0}^{n+1}\lambda_k^{-q,0}f(t_k^{-q,1}) \tag{5.3}$$

holds, where

$$t_k^{-q,1}=\frac{t}{2}\big(\xi_k^{-q,1}+1\big).$$

The relationship (1.3) leads to

$${}_0D_t^q f(t)\approx {}_0D_{t,n}^q f(t):=\frac{f(0)}{t^q\Gamma(1-q)}+D_{\star,n}^q f(t). \tag{5.4}$$

6. Numerical examples

In this section, we present some numerical experiments to illustrate and test the behavior of the approach described in the previous sections. In some examples the exact solutions of the fractional derivative can be expressed in terms of the Mittag-Leffler function of two parameters $E_{\alpha,\beta}(z)$, defined by the series expansion

$$E_{\alpha,\beta}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(k\alpha+\beta)}, \quad \alpha > 0,\ \beta \in \mathbb{R}. \tag{6.1}$$

The mathematical function `MittagLefflerE[alpha,beta,z]` is implemented in Mathematica and it is suitable for both symbolic and numerical calculation. Calculations in Matlab are considered in [13, 16, 37].

In our examples we consider the absolute error $e_n(f;t)$ at the point t, defined by

$$e_n^q(t) \equiv e_n^q(f;t) = |\,{}_0D_t^q f(t) - {}_0D_{t,n}^q f(t)\,|, \tag{6.2}$$

where ${}_0D_{t,n}^q f(t)$ is numerical value obtained by (5.4). We use also the maximum of $e_n^q(t)$ taken over certain interval A, i.e.,

$$E_n^q \equiv E_n^q(f) = \max_{t\in A} e_n^q(f;t) = \max_{t\in A} |\,{}_0D_t^q f(t) - {}_0D_{t,n}^q f(t)\,|.$$

In numerical calculations in our examples, the usual set $A = (0,1]$ will be always replaced by a discrete set, viz. $\{t_j = j/1000,\ j = 1,2,\ldots,1000\}$. Thus,

$$\widetilde{E}_n^q \equiv \widetilde{E}_n^q(f) = \max_{1\le j\le 1000} |{}_0D_t^q f(t_j) - {}_0D_{t,n}^q f(t_j)|. \tag{6.3}$$

Example **6.1**. In order to show numerically that the quadrature rule (5.2) has an algebraic degree of exactness $2n+1$, we take two types of algebraic polynomials. The first are the shifted Jacobi polynomials $P_m^{(-q,0)}(2t-1)$ and the second ones are monomials t^γ, $0 < t \le 1$.

In the first case, the exact solution of the fractional derivative is

$${}_0D_t^q P_m^{(-q,0)}(2t-1) = \frac{m!\,t^{-q}}{\Gamma(m-q+1)} P_m^{(0,-q)}(2t-1).$$

Using the quadrature formula (5.3) for $n = 5$ and $q = 1/2$, and taking the sequence of Jacobi polynomials $\{P_m^{(-1/2,0)}(2t-1)\}_{m=0}^{12}$ we calculate the corresponding sequence $\{\widetilde{E}_n^q\}_{m=0}^{12}$:

$$\big\{0.\times 10^{-16}, 0.\times 10^{-17}, 0.\times 10^{-17}, 0.\times 10^{-17}, 0.\times 10^{-17}, 0.\times 10^{-17}, 0.\times 10^{-17},$$
$$0.\times 10^{-17}, 0.\times 10^{-17}, 0.\times 10^{-17}, 0.\times 10^{-17}, 0.\times 10^{-18}, 0.4335\big\},$$

from which we see that the algebraic degree of exactness is $d = 11$ that is predicted by Theorem **4.1**.

Similarly, we can conclude from the second case for $f(t) = t^\gamma$, for which

$$ {}_0D_t^q t^\gamma = \frac{\Gamma(1+\gamma)}{\Gamma(1+\gamma-q)} t^{\gamma-q}, \quad \gamma > -1. $$

The corresponding sequence $\widetilde{E}_n^q$ for $\gamma = 0, 1, \ldots, 12$ (the maximum of the errors on $(0, 1]$), defined by (6.3), with the same quadrature ($n = 5$ and $q = 1/2$), is

$$ \{0. \times 10^{-18}, 0. \times 10^{-19}, 0. \times 10^{-19}, 0. \times 10^{-19}, 0. \times 10^{-19}, 0. \times 10^{-19}, 0. \times 10^{-19}, \\ 0. \times 10^{-19}, 0. \times 10^{-19}, 0. \times 10^{-19}, 0. \times 10^{-18}, 0. \times 10^{-18}, 2.55 \times 10^{-7}\}. $$

Using the same quadrature ($q = 1/2$ and $n = 5$), the maximum of the errors $\widetilde{E}_n^{1/2}$ for $f(t) = t^\gamma$, when γ runs over $[1, 12]$, is presented in Figure 1 (left) in $\log_{10}$-scale. As we can see the quadrature formula is exact in the cases when γ is an positive integer less than 12. In the same figure we give also the corresponding graphics for cases when $n = 10$, $n = 15$ and $n = 20$. Notice that these quadratures are exact for $\gamma \in \{0, 1, \ldots, 2n+1\}$. The case $q = 9/10$ is corresponding graphics are presented in Figure 1 (right).

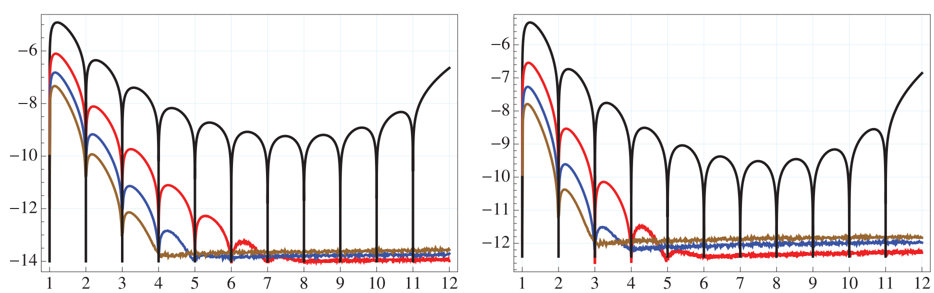

FIGURE 1. Maximum of $\log_{10} \widetilde{E}_n^q$ for $f(t) = t^\gamma$, $q = 1/2$ (left) and $q = 9/10$ (right), for quadratures with $n = 5(5)20$ nodes (graphics from top to bottom), when γ runs over interval $[1, 12]$

Now we consider the error $e_n^{1/2}(f; t)$, defined by (6.2), for a simple power function $f(t) = t^\gamma$ with an algebraic singularity. We take $\gamma = 1/2$, $3/2$, $7/2$, and $11/2$, and apply the Gauss-Lobatto quadratures (5.3) with $n = 5$, 10, 15, and 20 nodes (plus two fixed nodes at ± 1). The corresponding graphics in log-scale are presented in Figure 2.

As we can see the error $e_n^{1/2}(f; t)$ for a small γ ($= 1/2$) is almost constant for each t in the interval $(0, 1)$, but the convergence of the quadrature

γ	$n=5$	$n=10$	$n=15$	$n=20$	$n=30$	$n=60$	$n=90$	$n=120$
$\frac{1}{2}$	5.88(−4)	9.03(−5)	2.87(−5)	1.26(−5)	3.86(−6)	5.01(−7)	1.50(−7)	6.38(−8)
$\frac{1}{4}$	2.83(−3)	5.92(−4)	2.28(−4)	1.14(−4)	4.28(−5)	7.80(−6)	2.86(−6)	1.40(−6)
$\frac{1}{8}$	5.89(−3)	1.44(−3)	6.10(−4)	3.30(−4)	1.35(−4)	2.93(−5)	1.19(−5)	6.24(−6)
$\frac{1}{16}$	8.45(−3)	2.23(−3)	9.92(−4)	5.52(−4)	2.39(−4)	5.63(−5)	2.40(−5)	1.31(−5)

TABLE 1. Errors $e_n^{1/2}(f;1/2)$ in quadrature sums with $n=5(5)20$ and $n=30(30)120$, for $\gamma=1/2$, $1/4$, $1/8$, and $1/16$

formulas (5.3) is rather slow, especially when γ is closer to zero. For example, for $\gamma=1/2$, $1/4$, $1/8$, and $1/16$, the errors $e_n^{1/2}(f;t)$ at $t=1/2$ are given in Table 1 for quadrature rules with $n=5(5)20$ and $n=30(30)120$ nodes. Numbers in parentheses indicate decimal exponents. For $\gamma>1$ the convergence is satisfactory.

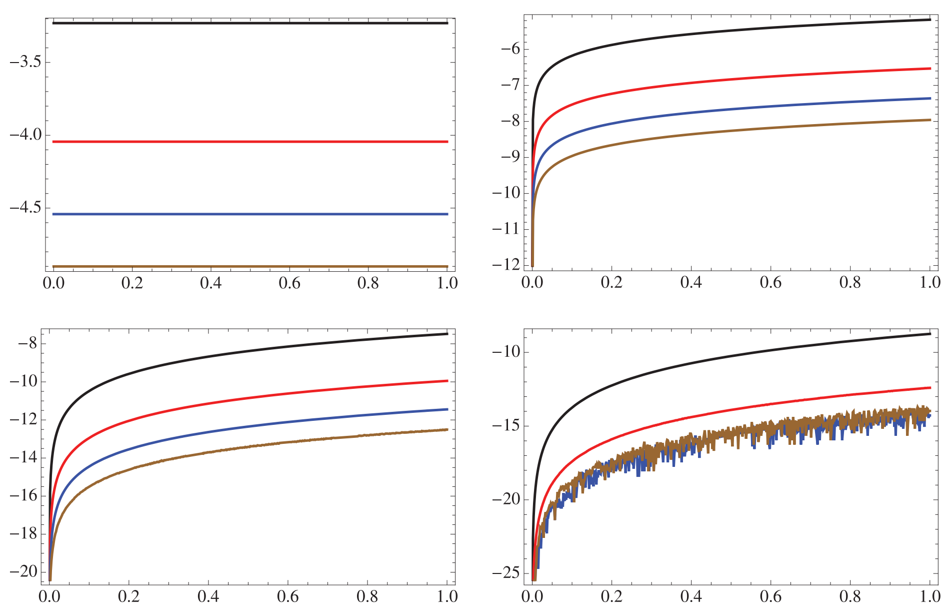

FIGURE 2. Graphics of $\log_{10} e_n^q(f;t)$ for $f(t)=t^\gamma$ and t runs over $(0,1)$, when $n=5(5)20$ (graphics from top to bottom) in the cases: (above) $\gamma=1/2$ (left) and $\gamma=3/2$ (right); (below) $\gamma=7/2$ (left) and $\gamma=11/2$ (right)

Remark **6.1**. Problems with algebraic or/and logarithmic singularities can be solved using Müntz systems and quadratures of this type (cf. [30, 32, 11]) or using a procedure proposed in [20].

Example **6.2**. For our second experiment we consider fractional differentiation by ploting $\sin(t)$ on the interval $[0, 4\pi]$ (already used in [19]), together with its derivatives of order $q = 1/10, 2/10, \ldots, 9/10$, as drawn in Figure 3. Fractional derivatives have been calculated using the quadrature rule (5.3) with $n = 5$. As one can see, each curve is approximately a translation of $\sin(t)$ by a distance $q\pi/2$ to the left.

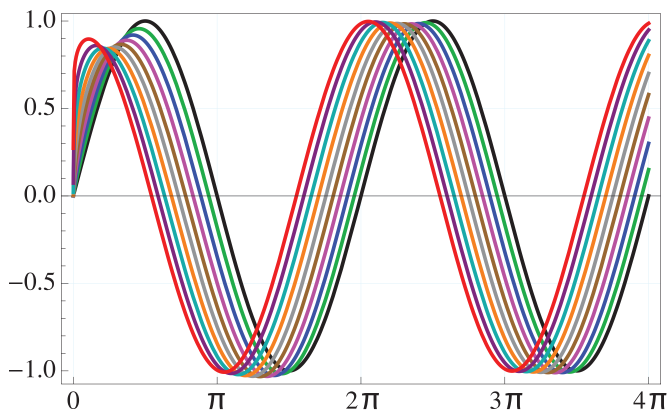

Figure 3. The function $\sin(t)$ on $[0, 4\pi]$ together with its derivatives of order $k/10$, $k = 1, 2, \ldots, 9$

Example **6.3**. We compute ${}_0D_t^q f(t)$ for $f(t) = \sin(\lambda t)$ and $t \in [0, \pi]$. The exact value of the fractional derivative of this function is given by [39, 41]

$$ {}_0D_t^q \sin(\lambda t) = \lambda t^{1-q} E_{2,2-q}(-\lambda^2 t^2), $$

where the Mittag-Leffler function is defined in (6.1).

In Figure 4 we present graphics of the functions $\sin(\lambda x)$, $\lambda = 1, 2, 3$ (left), and their derivatives of order $q = 1/2$ (right), obtained by the Gauss-Lobatto quadrature rule (5.3) with $n = 5$ internal nodes. Since the sin-function is smooth, this quadrature rule converges very fast. In order to illustrate this fact we present in Table 2 the numerical results ${}_0D_{t,n}^q \sin(\lambda t)$ for $t = \pi/2$, $q = 1/2$, $\lambda = 2$ and $\lambda = 3$, taking $n = 2(1)8$ internal nodes in the Gauss-Lobatto quadrature rule (5.3), as well as the corresponding

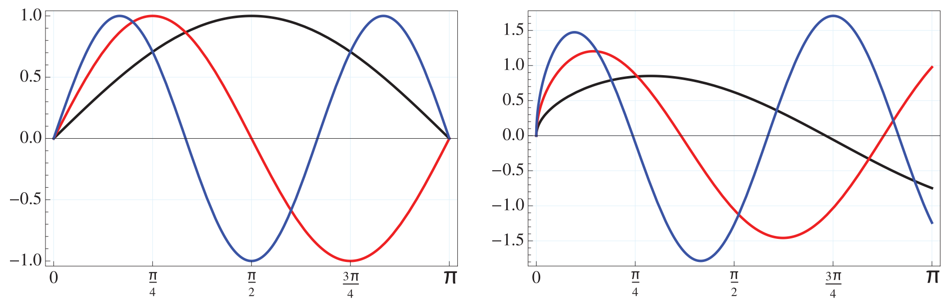

FIGURE 4. Graphics of the functions $\sin(\lambda x)$, $\lambda = 1, 2, 3$ (left), and their derivatives obtained by the numerical quadrature (5.3) with $n = 5$ (right)

n	${}_0D^q_{t,n} \sin(2t)$	$r^q_n(2;t)$	${}_0D^q_{t,n} \sin(3t)$	$r^q_n(3;t)$
2	−1.05**6**8638589376709	8.69(−4)	−1.26**4**0813951622687	2.41(−3)
3	−1.0577**9**33376552489	9.59(−6)	−1.267**2**323502405542	7.79(−5)
4	−1.0577831**2**05699668	6.58(−8)	−1.26713**1**8332287842	1.39(−6)
5	−1.057783190**5**482818	3.08(−10)	−1.267133**6**100910347	1.59(−8)
6	−1.05778319022**1**3884	1.04(−12)	−1.267133589**7**303999	1.29(−10)
7	−1.05778319022249**6**0	2.69(−15)	−1.26713358989**5**1450	7.81(−13)
8	−1.057783190222493**2**	5.41(−18)	−1.26713358989415**0**1	3.67(−15)

TABLE 2. Gaussian approximations ${}_0D^q_{t,n} \sin(\lambda t)$ and the corresponding relative errors $r^q_n(\lambda;t)$ for $f(t) = \sin(\lambda t)$ and $q = 1/2$ at $t = \pi/2$

relative errors

$$r^q_n(\lambda;t) = \left| \frac{{}_0D^q_{t,n} \sin(\lambda t) \; - \; {}_0D^q_t \sin(\lambda t)}{{}_0D^q_t \sin(\lambda t)} \right| .$$

In each entry the first digit in error is bolded and underlined.

The maximal absolute errors in Gaussian approximations over the whole interval $(0, \pi)$ (taking 1000 equidistant points $t_j = j\pi/1000$, $j = 1, \dots, 1000$) are presented in Table 3.

EXAMPLE **6.4**. We compute ${}_0D^q_t f(t)$ for $f(t) = (t+\nu)^{q-1}$ and $t \in [0, 1]$. The exact value of the fractional derivative of this function is given by [39]

$${}_0D^q_t (t+\nu)^{q-1} = \frac{1}{\Gamma(1-q)} \left(\frac{\nu}{t}\right)^q \frac{1}{t+\nu}.$$

n	4	6	8	10	12
$\lambda = 1$	4.93(−8)	7.81(−13)	4.05(−18)		
$\lambda = 2$	1.73(−5)	3.42(−9)	2.32(−13)	6.80(−18)	
$\lambda = 3$	1.50(−3)	2.41(−6)	1.13(−9)	2.12(−13)	1.91(−17)

TABLE 3. Maximal absolute errors in Gaussian approximations ${}_0D^q_{t,n}\sin(\lambda t)$, when $t \in (0, \pi]$, $q = 1/2$, $\lambda = 1, 2, 3$ and $n = 4(2)12$

The actual maximum error $\widetilde{E}^q_n$, defined by (6.3), is plotted in Figure 5 in a semi-log coordinate system as a function of n for $q = 1/2$ and four values of the parameter ν (= 0.1, 0.2, 0.5 and 1.0).

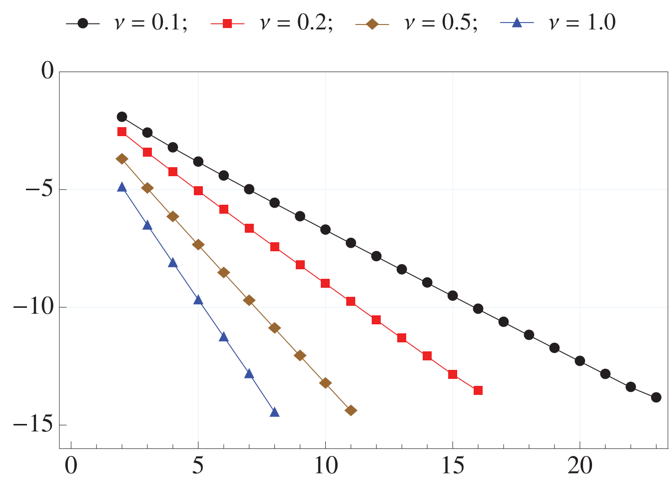

FIGURE 5. $\log_{10}\widetilde{E}^q_n$ versus n for $q = 1/2$ with $\nu = 0.1, 0.2, 0.5, 1.0$

As we can see that $\widetilde{E}^q_n$ decreases rapidly. It is worth noting that the convergence rate is dependent of the regularity of the integrand in the neighborhood of $t = 0$. As one can see, in the case that ν tends to zero, the quadrature rule converges slowly.

EXAMPLE **6.5**. For exponential functions $f_1(t;\lambda) = \mathrm{e}^{\lambda t}$ and $f_2(t;\lambda) = \cosh(\sqrt{\lambda}\,t)$, $t \in [0, 1]$, the exact values of the fractional derivative ${}_0D^q_t f_k(t;\lambda)$, $k = 1, 2$, are given in terms of the Mittag-Leffler function (6.1) (cf. [36, 41]) as

$$ {}_0D^q_t\mathrm{e}^{\lambda t} = t^{-q}E_{1,1-q}(\lambda t) $$

	n	4	6	8	10
f_1	$\lambda = 1/2$	1.28(−10)	1.20(−16)		
	$\lambda = 1$	3.32(−7)	4.81(−12)	2.36(−17)	
	$\lambda = 2$	2.36(−3)	4.49(−7)	3.71(−11)	1.20(−15)
f_2	$\lambda = 1/2$	3.25(−9)	1.21(−14)	1.51(−20)	
	$\lambda = 1$	1.71(−7)	2.48(−12)	1.22(−17)	
	$\lambda = 2$	1.18(−5)	6.59(−10)	1.27(−14)	1.05(−19)

TABLE 4. Maximal absolute errors $\widetilde{E}_n^q(f_k)$, $k = 1, 2$, $\lambda = 1/2, 1, 2$, over $(0, 1]$, in Gaussian approximations for $q = 1/2$, with $n = 4(2)10$ internal nodes

and

$$ {}_0D_t^q \cosh(\sqrt{\lambda}\, t) = t^{-q} E_{2,1-q}(\lambda t^2). $$

The maximal absolute errors in Gaussian approximations $\widetilde{E}_n^q(f_k)$, $k = 1, 2$, over the whole interval $(0, 1)$, defined by (6.3), are presented in Table 4.

EXAMPLE **6.6**. Finally, we compute ${}_0D_t^q f(t)$ for $f(t) = t^{a/2} J_a\big(2\sqrt{t}\big)$ and $t \in [0, 1]$, where $J_a(z)$ is the Bessel function of the first kind and order a, defined as a solution of the so-called Bessel differential equation

$$ z^2 \frac{\mathrm{d}^2 y}{\mathrm{d}z^2} + z\frac{\mathrm{d}y}{\mathrm{d}z} + (z^2 - a^2)y = 0, $$

which can be expressed in the power form expansion around $z = 0$,

$$ J_a(z) = \sum_{k=0}^{\infty} \frac{(-1)^k}{k!\Gamma(k + a + 1)} \Big(\frac{z}{2}\Big)^{2k+a}. $$

The exact value of the fractional derivative of this function is given by [36, 41]

$$ {}_0D_t^q f(t) = t^{(a-q)/2} J_{a-q}\big(2\sqrt{t}\big), $$

Since the original function

$$ f(t) = f(t; a) = t^{a/2} J_a\big(2\sqrt{t}\big) = \sum_{k=0}^{\infty} \frac{(-1)^k}{k!\Gamma(k + a + 1)} t^{k+a}, $$

we see that f is an analytic function when $a \in \mathbb{N}_0$, so that for such values of the parameter a we expect fast convergence of the quadrature rule (5.3). However, in other cases this function has an algebraic singularity at $t = 0$.

As a decreases to zero, the convergence of our quadrature rule slows down considerably. In Figure 6 we present graphics of the maximal error $\widetilde{E}_n^q(f(\,\cdot\,; a))$ for $q = 1/2$, obtained by three different quadrature rules with

$n = 5$, 10, and 20 internal nodes, when the parameter a in the function runs over $(0, 3.5)$. It is clear that the rapidly increasing of accuracy achieved when the parameter a tends to an integer, i.e., when f becomes an analytic function.

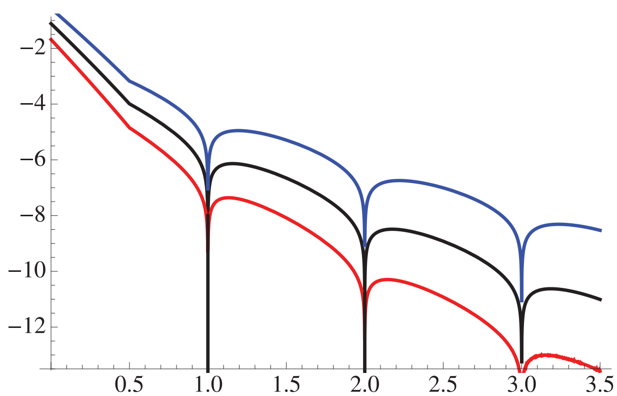

FIGURE 6. Graphics of $\log_{10}[\widetilde{E}_n^{1/2}(f(\cdot\,;a))]$ for $n = 5$, 10, and 20 (from top to bottom), when $0 < a < 3.5$

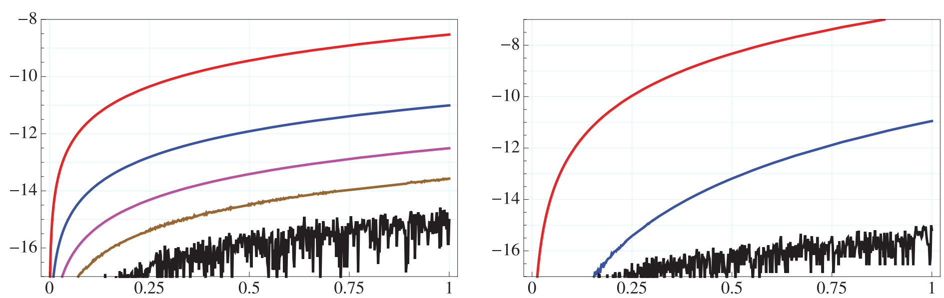

FIGURE 7. The values $\log_{10}[e_n^{1/2}(f;t)]$, $0 < t < 1$, for $n = 2, 3, 4$ internal nodes (graphics from top to bottom), when $a = 2$ (left) and $a = 3$ (right)

Thus, for $a \in \mathbb{N}_0$ the convergence of the quadrature rule (5.3) is very fast! The errors $e_n^{1/2}(f;t)$, $0 < t < 1$, in approximation of fractional derivative ${}_0D_t^q f(t)$ by quadrature rules with a small number of nodes ($n = 2, 3, 4$) are presented in Figure 7 (in log-scale) for $a = 2$ (left) and $a = 3$ (right).

On the other side, taking much more nodes (up to $n = 120$), for a small a, viz. $a = 1/2$, the convergence is very slow (see Figure 8 (left)). Something faster convergence is achieved for $a = 3/2$ (Figure 8 (right)).

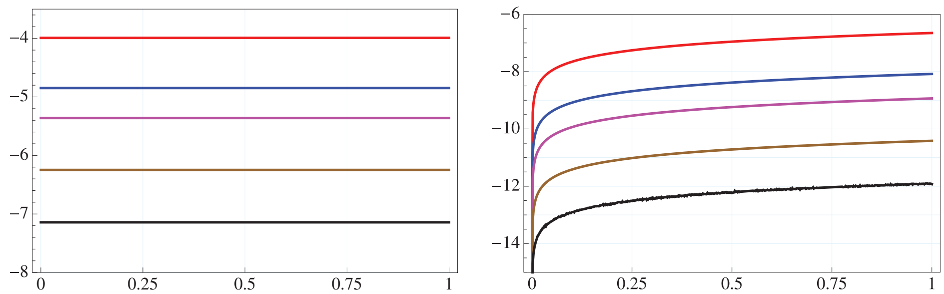

FIGURE 8. The values $\log_{10}[e_n^{1/2}(f;t)]$, $0 < t < 1$, for $n = 10, 20, 30, 60, 120$ internal nodes (graphics from top to bottom), when $a = 1/2$ (left) and $a = 3/2$ (right)

However, if a is sufficiently large the convergence rate becomes quite satisfactory, as is given in Figure 9 (left) for $a = 7/2$, where we used $n = 5(5)20$ and $n = 30$ internal nodes in the corresponding quadrature rule (5.3).

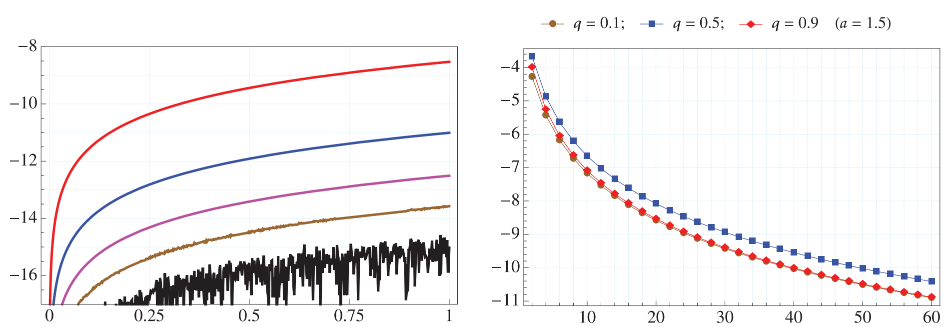

FIGURE 9. (left) The values $\log_{10}[e_n^{1/2}(f;t)]$, $0 < t < 1$, $a = 7/2$, for $n = 5, 10, 15, 20, 30$ internal nodes (graphics from top to bottom); (right) $\log_{10}[\widetilde{E}_n^q(f(\,\cdot\,;a))]$, $a = 3/2$, versus n for $q = 1/10$, $1/2$, and $9/10$

Finally, in Figure 9 (right) we present the actual maximum error $\widetilde{E}_n^q(f)$, defined by (6.3), in a semi-log coordinate system as a function of n for $a = 3/2$ and three values of q ($= 1/10$, $1/2$, and $9/10$). As we can see the behaviour of $\widetilde{E}_n^q(f)$ is very similar with respect to q.

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