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ORIGINAL PAPER

An investigation of some nonclassical methods for the numerical approximation of Caputo-type fractional derivatives

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Abstract Traditional methods for the numerical approximation of fractional derivatives have a number of drawbacks due to the non-local nature of the fractional differential operators. The main problems are the arithmetic complexity and the potentially high memory requirements when they are implemented on a computer. In a recent paper, Yuan and Agrawal have proposed an approach for operators of order $\alpha \in (0, 1)$ that differs substantially from the standard methods. We extend the method to arbitrary $\alpha > 0, \alpha \notin \mathbb{N}$, and give an analysis of the main properties of this approach. In particular it turns out that the original algorithm converges rather slowly. Based on our analysis we are able to identify the source of this slow convergence and propose some modifications leading to a much more satisfactory behaviour. Similar results are obtained for a closely related method proposed by Chatterjee.

Keywords Fractional derivatives · Caputo derivative · Numerical approximation · Yuan-Agrawal method · Fractional differential equation

Mathematics Subject Classifications (2000) Primary 65D25 · Secondary 26A33 · 65L05

Dedicated to Professor Paul L. Butzer on the occasion of his 80th birthday.

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1 Introduction

Caputo-type fractional differential operators of order $\alpha > 0$ with $\alpha \notin \mathbb{N}$, denoted and defined by

$$D_*^\alpha y(x) := \frac{1}{\Gamma(\lceil\alpha\rceil - \alpha)} \int_0^x (x-\tau)^{\lceil\alpha\rceil-\alpha-1} y^{(\lceil\alpha\rceil)}(\tau)\, d\tau, \tag{1}$$

have proven to be important tools in the mathematical modeling of many phenomema in physics and engineering, see, e.g., [1, 3, 8, 12, 14, 17] and the references cited therein. Here and in the following, $\lceil\cdot\rceil$ denotes the ceiling function that rounds up to the nearest integer not less than its argument, whereas later on we shall also use the floor function $\lfloor\cdot\rfloor$ that rounds down to the nearest integer not exceeding its argument. A particularly important case in many applications is $0 < \alpha < 1$. In this situation, (1) reduces to

$$D_*^\alpha y(x) = \frac{1}{\Gamma(1-\alpha)} \int_0^x (x-\tau)^{-\alpha} y'(\tau) d\tau. \tag{2}$$

Even though many authors restrict their attention to this special case, it will turn out that our methods can handle the fully general problem where α may be an arbitrary positive non-integer.

In view of the large number of potential applications of such operators (some of which have been mentioned above) it is evident that there is a substantial demand for efficient schemes for their numerical handling. A number of methods for the solution of this problem have been proposed in the recent decades, see, e.g., [7, 9, 15, 16]. A common feature of all these methods is that they essentially all deal with the non-locality of the operator (i.e. with the fact that information about the function y on the entire interval $[0, x]$ is required in order to compute $D_*^\alpha y(x)$, which is a fundamental difference to the classical differential operator of integer order that only needs data from a small neighbourhood of the point x) in the same way, namely by sampling the function y (or y') on a more or less regular grid in $[0, x]$. In a typical application, one needs to find approximations for $D_*^\alpha y(x)$ for x in a certain interval $[0, X]$, say, i.e. one has to compute these approximations for many different values of x. Since each of these computations is expensive in terms of (a) run time for the function evaluations and the arithmetic operations to be carried out with the function values and (b) memory required for storing those function values that are needed more than once, the complete process is very expensive.

At present, three concepts have been proposed in an attempt to reduce this high computational cost. Two of these concepts have been investigated thoroughly. The first one is the "short memory principle" of Podlubny [17, § 7.3]. It states that one should simply ignore all contributions coming from points that are more than a preassigned threshold T, say, away from the presently considered point x. This principle leads to a very cheap algorithm but, as shown in [10], its approximation properties are poor. As an alternative, Ford and Simpson [10] have suggested a so-called "logarithmic memory principle". This means that the mesh spacing is very fine near the current point x and becomes

coarser as we move away from this point. When implemented properly, this approach can lead to an arithmetic complexity that is only marginally higher than in the case of integer-order (i.e. local) operators without losing the convergence order of the method. A full description of this approach and its properties is given in [10].

Much less is known about the behaviour of the third method. It has been proposed by Yuan and Agrawal [24] who follow a completely different path in its development. Whereas the complexity of the algorithm is quite evident [14, 19, 24], reports on the quality of the results produced by this method in practical applications give a rather unclear picture. It seems that some authors have been able to use it successfully [18, 23, 24] whereas others criticize it strongly [14, 19] and support their point of view by arguments based on the mechanical interpretation of the approach [19]. A theoretical investigation of the accuracy and other fundamental properties of this method does not seem to be available. We therefore aim to provide insight into the approach by analyzing it from a mathematical perspective, thus filling this void. Our main emphasis will be on the convergence behaviour, but we shall also address its computational aspects.

In order to achieve our goals, we will proceed as follows. In the next section, we recall the precise definition of the Yuan-Agrawal method. At the same time we demonstrate how to extend it to the case $\alpha > 1$. Section 3 is be devoted to a convergence analysis. Based on these investigations we provide improved versions of the algorithm in Sections 4 and 5, and then we continue the paper with a section with numerical experiments that clearly show the superiority of the modified approach. Finally, we summarize our findings in Section 7.

2 The Yuan-Agrawal method and its basic properties

Let us first recall the details of the method proposed by Yuan and Agrawal [24]. In this context we note that Yuan and Agrawal have only discussed the case $0 < \alpha < 1$. An extension to $1 < \alpha < 2$ has been provided by Trinks and Ruge [23]. However, we shall see below that it is possible to extend the approach and the following analysis to the general case of arbitrary positive $\alpha \notin \mathbb{N}$. Therefore we will not impose any restriction on the size of α. It can easily be seen that our approach reduces to the original scheme of Yuan and Agrawal if $0 < \alpha < 1$.

2.1 The analytical background of the fundamental idea

To describe the approach completely, we assume our function $y \in C^{\lceil\alpha\rceil}[0, X]$ in (1) and the order $\alpha > 0, \alpha \notin \mathbb{N}$, of the differential operator to be given. Then we define an auxiliary bivariate function $\phi : (0, \infty) \times [0, X] \to \mathbb{R}$ by

$$\phi(w, x) := (-1)^{\lfloor\alpha\rfloor} \frac{2 \sin \pi\alpha}{\pi} w^{2\alpha - 2\lceil\alpha\rceil + 1} \int_0^x y^{(\lceil\alpha\rceil)}(\tau) e^{-(x-\tau)w^2} \, d\tau. \tag{3}$$

With this notation we obtain the following generalization of a result of [24, Section 2]:

Theorem 1 *Under the above assumptions,*

$$D_*^\alpha y(x) = \int_0^\infty \phi(w,x)\,dw. \tag{4}$$

In addition, for fixed $w > 0$ the function $\phi(w,\cdot)$ satisfies the differential equation

$$\frac{\partial}{\partial x}\phi(w,x) = -w^2\phi(w,x) + (-1)^{\lfloor\alpha\rfloor}\frac{2\sin\pi\alpha}{\pi}w^{2\alpha-2\lceil\alpha\rceil+1}y^{(\lceil\alpha\rceil)}(x) \tag{5}$$

subject to the initial condition $\phi(w,0) = 0$.

Notice that the differential equation (5) is effectively an ordinary differential equation since we assume w to be a fixed parameter. Moreover it is a differential equation of order 1 and hence of classical (not fractional in the strict sense) type. In addition we note that the differential equation is linear and inhomogeneous and that it has constant coefficients. Therefore it is a simple matter to compute the solution of the initial value problem explicitly, and of course this computation reproduces the representation (3).

Proof of Theorem 1 Bearing in mind the well known facts that

$$\Gamma(u) = \int_0^\infty e^{-z}z^{u-1}\,dz \qquad (u > 0),$$

$$\Gamma(u)\Gamma(1-u) = \frac{\pi}{\sin\pi u} \qquad (0 < u < 1)$$

and

$$\sin\pi(\alpha - \lceil\alpha\rceil + 1) = (-1)^{\lfloor\alpha\rfloor}\sin\pi\alpha \qquad (\alpha \notin \mathbb{N})$$

we obtain from (1) that

$$\begin{aligned}
D_*^\alpha y(x) &= \frac{1}{\Gamma(\lceil\alpha\rceil-\alpha)}\int_0^x (x-\tau)^{\lceil\alpha\rceil-\alpha-1}y^{(\lceil\alpha\rceil)}(\tau)\,d\tau \\
&= \frac{1}{\Gamma(\alpha-\lceil\alpha\rceil+1)\Gamma(\lceil\alpha\rceil-\alpha)} \\
&\quad\times\int_0^x\int_0^\infty e^{-z}z^{\alpha-\lceil\alpha\rceil}\,dz\,(x-\tau)^{\lceil\alpha\rceil-\alpha-1}y^{(\lceil\alpha\rceil)}(\tau)\,d\tau \\
&= \frac{\sin\pi(\alpha-\lceil\alpha\rceil+1)}{\pi}\int_0^x\int_0^\infty e^{-z}\left(\frac{z}{x-\tau}\right)^{\alpha-\lceil\alpha\rceil+1}\frac{1}{z}y^{(\lceil\alpha\rceil)}(\tau)\,dz\,d\tau \\
&= (-1)^{\lfloor\alpha\rfloor}\frac{\sin\pi\alpha}{\pi}\int_0^x\int_0^\infty e^{-z}\left(\frac{z}{x-\tau}\right)^{\alpha-\lceil\alpha\rceil+1}\frac{1}{z}y^{(\lceil\alpha\rceil)}(\tau)\,dz\,d\tau.
\end{aligned}$$

We may now apply the substitution $z = (x-\tau)w^2$ in the inner integral and note that Fubini's Theorem allows us to interchange the order of the integrations since $y^{(\lceil\alpha\rceil)}$ is assumed to be continuous. This yields

$$D_*^\alpha y(x) = (-1)^{\lfloor\alpha\rfloor}\frac{2\sin\pi\alpha}{\pi}\int_0^x\int_0^\infty e^{-(x-\tau)w^2}w^{2\alpha-2\lceil\alpha\rceil+1}y^{(\lceil\alpha\rceil)}(\tau)\,dw\,d\tau$$

$$= \int_0^\infty (-1)^{\lfloor\alpha\rfloor}\frac{2\sin\pi\alpha}{\pi}w^{2\alpha-2\lceil\alpha\rceil+1}\int_0^x e^{-(x-\tau)w^2}y^{(\lceil\alpha\rceil)}(\tau)\,d\tau\,dw$$

and, recalling the definition (3) of ϕ, we deduce (4).

Next we differentiate the definition (3) of ϕ with respect to x. The classical rules for the differentiation of parameter integrals with respect to the parameter immediately give (5). Finally the fact that $\phi(w,0) = 0$ for $w > 0$ is also a direct consequence of (3) because the integrand of the integral on the right-hand side of (3) is continuous. □

At this point we want to mention a closely related approach recently proposed by Chatterjee [4] (see also [21]). As we have seen above, the Yuan-Agrawal approach is based on expressing the fractional derivative of the given function y in the form of an integral over $(0,\infty)$, cf. Eq. 4, whose integrand can be computed as the solution of first-order initial value problem (5). This feature is shared by Chatterjee's method. Specifically, it is based on the following analogue of Theorem 1. The result essentially states that we may replace the integrand ϕ by a function ϕ^* which can be characterized as the solution of a different first-order initial value problem.

Theorem 2 *For fixed $w > 0$, let $\phi^*(w,\cdot)$ be the solution of the differential equation*

$$\frac{\partial}{\partial x}\phi^*(w,x) = -w^{1/(\alpha-\lceil\alpha\rceil-1)}\phi^*(w,x) + \frac{(-1)^{\lfloor\alpha\rfloor}\sin\pi\alpha}{\pi(\alpha-\lceil\alpha\rceil+1)}y^{(\lceil\alpha\rceil)}(x) \tag{6}$$

subject to the initial condition $\phi^*(w,0) = 0$. Then, we have

$$\phi^*(w,x) = \frac{(-1)^{\lfloor\alpha\rfloor}\sin\pi\alpha}{\pi(\alpha-\lceil\alpha\rceil+1)}\int_0^x y^{(\lceil\alpha\rceil)}(\tau)\exp\left(-(x-\tau)w^{1/(\alpha-\lceil\alpha\rceil+1)}\right)d\tau \tag{7}$$

and

$$D_*^\alpha y(x) = \int_0^\infty \phi^*(w,x)\,dw. \tag{8}$$

The proof of this result is almost identical to the proof of Theorem 1; one only needs to replace the substitution $z = (x-\tau)w^2$ by $z = (x-\tau)w^{1/(\alpha-\lceil\alpha\rceil+1)}$ and use the functional equation of the Gamma function, $u\Gamma(u) = \Gamma(u+1)$. We leave the details to the reader.

It seems that this approach has not received as much attention from the point of view of applications yet, so we will be rather brief in its discussion. We do stress however that the entire theory that we shall develop for the original

Yuan-Agrawal method based on Theorem 1 can easily be applied to Chatterjee's variant of the method as well.

2.2 The numerical part of the method

Based on Theorem 1, Yuan and Agrawal [24, Section 3] suggest to proceed in two steps in order to construct the desired approximation for the fractional derivative $D_*^\alpha y(x)$. Their algorithm uses two parameters $h > 0$ and $n \in \mathbb{N}$ whose values are assumed to be given by the user. Then, the construction works as follows.

In the first step, let $z_{kn}^{(\gamma)}$ be the kth zero of the Laguerre polynomial of degree n ($k = 1, 2, \ldots, n$) with respect to the weight function $w^\gamma e^{-w}$, where we assume the ordering

$$z_{1n}^{(\gamma)} < z_{kn}^{(\gamma)} < \cdots < z_{nn}^{(\gamma)}.$$

(We shall comment on the choice of the parameter γ later.) Then, Yuan and Agrawal compute an approximate solution $\phi_h\left(z_{kn}^{(\gamma)}, x\right)$ of the differential equation (5) for all k and for those values of x for which an approximate value of $D_*^\alpha y(x)$ is desired. In principle, any numerical algorithm with step size h may be used to solve the differential equation (e.g., a Runge-Kutta scheme or a linear multistep method) if h is sufficiently small. For details, especially with respect to the meaning of the restriction "if h is sufficiently small", we refer to Sections 3.2 and 6. We point out here in particular that, by using the differential equation (5), this approach avoids to use the definition (3) of ϕ explicitly.

The second step performs the actual computation of the fractional derivative by means of Eq. 4. However, instead of using the exact function ϕ in the integral on the right-hand side of (4), we use the approximation ϕ_h that we have just computed. The integration itself is also done numerically. To this end, Yuan and Agrawal propose to write

$$\int_0^\infty \phi_h(w, x)dw = \int_0^\infty w^\gamma e^{-w}\left[w^{-\gamma}e^w\phi_h(w, x)\right]dw$$

and to use a generalized Gauss-Laguerre quadrature formula $Q_n^{\mathrm{GL}\gamma}$ for the weight function $w^\gamma e^{-w}$ with n integration points [6] with respect to the factor in brackets, thus obtaining

$$D_{n,h}^\alpha y(x) := \sum_{k=1}^{n} w_{kn}^{(\gamma)} \left(z_{kn}^{(\gamma)}\right)^{-\gamma} e^{z_{kn}^{(\gamma)}} \phi_h\left(z_{kn}^{(\gamma)}, x\right), \tag{9}$$

with $w_{kn}^{(\gamma)}$ denoting the (generalized) Laguerre weights, as the final approximation for $D_*^\alpha y(x)$. Specifically, Yuan and Agrawal suggest to use $\gamma = 0$; we shall see in Section 3.1 that other choices may be more appropriate.

We are mainly interested in the investigation of the error of this approximation method as the parameters n (the number of integration points in the Laguerre formula) and h (the step size of the differential equation solver) vary. Actually we have a third parameter, namely the value γ that precisely defines

the weight function. This parameter will always be kept fixed, and therefore we have omitted it from the notation $D^{\alpha}_{n,h}y(x)$ introduced for the numerical approximation in Eq. 9.

Because of the way in which the construction is divided into the two steps, it is evident that the complete error analysis for the algorithm needs to take into account both the error introduced by the Laguerre quadrature and the error introduced by the differential equation solver. To be precise, the error $R^{\alpha}_{n,h}y(x)$ is given by

$$\begin{aligned} R^{\alpha}_{n,h}y(x) &:= D^{\alpha}_{*}y(x) - D^{\alpha}_{n,h}y(x) \\ &= \int_0^{\infty} \phi(w,x)\,dw - \sum_{k=1}^{n} w^{(\gamma)}_{kn}\left(z^{(\gamma)}_{kn}\right)^{-\gamma} e^{z^{(\gamma)}_{kn}}\phi_h\left(z^{(\gamma)}_{kn},x\right) \\ &= R^{\mathrm{GL}\gamma}_{n}\left[(\cdot)^{-\gamma}\exp(\cdot)\phi(\cdot,x)\right] + Q^{\mathrm{GL}\gamma}_{n}\left[(\cdot)^{-\gamma}\exp(\cdot)E_h(\cdot,x)\right] \end{aligned} \tag{10}$$

where

$$R^{\mathrm{GL}\gamma}_{n}\left[(\cdot)^{-\gamma}\exp(\cdot)\phi(\cdot,x)\right] := \int_0^{\infty}\phi(w,x)\,dw - \sum_{k=1}^{n} w^{(\gamma)}_{kn}\left(z^{(\gamma)}_{kn}\right)^{-\gamma} e^{z^{(\gamma)}_{kn}}\phi\left(z^{(\gamma)}_{kn},x\right) \tag{11}$$

denotes the error of the Gauss-Laguerre quadrature and

$$E_h(w,x) := \phi(w,x) - \phi_h(w,x) \tag{12}$$

is the error of the differential equation solver.

We shall discuss these quantities in Section 3.

3 Error analysis of the Yuan-Agrawal method

From Eqs. 10, 11 and 12, it is clear that we may discuss the two components of the error separately. The combination of the results will then produce the final error bound.

3.1 The contribution of the Gauss-Laguerre formula

We begin our investigation with the error of the Gauss-Laguerre quadrature given in (11). It has been observed elsewhere [14, Section 3] that the convergence behaviour of the Laguerre scheme can be very slow. From the point of view of approximation theory, this phenomenon can be explained. For this purpose, it is useful to look at the asymptotic behaviour of the integrand in (4) as the integration variable w converges to one of the end points of the interval of integration. Here and in the following, the symbol $a(v) \sim b(v)$ means that there exist two strictly positive constants A and B such that $|a(v)/b(v)| \in [A, B]$ as v tends to the indicated limit.

Theorem 3 *Let $x \in (0, X)$ be fixed and $0 < \alpha \notin \mathbb{N}$, and assume that there exists some $C > 0$ such that $|y^{(\lceil\alpha\rceil)}(\tilde{x})| > C$ for all $\tilde{x} \in [0, X]$.*

(a) *The function $\phi(\cdot, x)$ defined in (3) behaves as*

$$\phi(w, x) \sim w^{2\alpha-2\lceil\alpha\rceil+1} \quad \text{as } w \to 0. \tag{13}$$

(b) *Moreover,*

$$\phi(w, x) \sim w^{2\alpha-2\lceil\alpha\rceil-1} \quad \text{as } w \to \infty. \tag{14}$$

(c) *We have $\phi(\cdot, x) \in C^\infty(0, \infty)$.*

Remark 1 The condition that $y^{(\lceil\alpha\rceil)}$ be bounded away from zero is a technical condition required in order to keep the proof simple and to keep the result valid for *all* $x \in (0, X)$. Using more complicated techniques, one could show that the same asymptotic behaviour is present for *almost all* $x \in (0, X)$ under substantially weaker conditions. Thus it is justified to say that the asymptotic behaviour described in Theorem 3 is the behaviour that one may reasonably expect for the function ϕ unless the given function y is of a highly exceptional nature.

Proof of Theorem 3 For part (a), a partial integration gives

$$\begin{aligned}
&\int_0^x y^{(\lceil\alpha\rceil)}(\tau)e^{-(x-\tau)w^2}\,d\tau \\
&\quad = y^{(\lceil\alpha\rceil-1)}(\tau)e^{-(x-\tau)w^2}\Big|_{\tau=0}^{\tau=x} - w^2\int_0^x y^{(\lceil\alpha\rceil-1)}(\tau)e^{-(x-\tau)w^2}\,d\tau \\
&\quad = y^{(\lceil\alpha\rceil-1)}(x) - y^{(\lceil\alpha\rceil-1)}(0)e^{-xw^2} - w^2\int_0^x y^{(\lceil\alpha\rceil-1)}(\tau)e^{-(x-\tau)w^2}\,d\tau.
\end{aligned}$$

Since x is fixed, the rightmost integral obviously remains bounded as $w \to 0$, and hence we conclude

$$\lim_{w\to 0}\int_0^x y^{(\lceil\alpha\rceil)}(\tau)e^{-(x-\tau)w^2}\,d\tau = y^{(\lceil\alpha\rceil-1)}(x) - y^{(\lceil\alpha\rceil-1)}(0). \tag{15}$$

Inserting this relation into the definition (3) of ϕ we obtain the first claim.

For the proof of (b), we write

$$\begin{aligned}
&w^2\int_0^x y^{(\lceil\alpha\rceil)}(\tau)e^{-(x-\tau)w^2}\,d\tau \\
&\quad = w^2\int_0^{x-w^{-1}} y^{(\lceil\alpha\rceil)}(\tau)e^{-(x-\tau)w^2}\,d\tau + w^2\int_{x-w^{-1}}^x y^{(\lceil\alpha\rceil)}(\tau)e^{-(x-\tau)w^2}\,d\tau \\
&\quad = y^{(\lceil\alpha\rceil)}(\xi_1)w^2\int_0^{x-w^{-1}} e^{-(x-\tau)w^2}\,d\tau + y^{(\lceil\alpha\rceil)}(\xi_2)w^2\int_{x-w^{-1}}^x e^{-(x-\tau)w^2}\,d\tau \\
&\quad = y^{(\lceil\alpha\rceil)}(\xi_1)(e^{-w} - e^{-w^2}) + y^{(\lceil\alpha\rceil)}(\xi_2)(1 - e^{-w})
\end{aligned}$$

with some $\xi_1 \in [0, x - w^{-1}]$ and $\xi_2 \in [x - w^{-1}, x]$ because of the Mean Value Theorem. Now, as $w \to \infty$, $y^{(\lceil\alpha\rceil)}(\xi_1)$ remains bounded whereas $e^{-w} - e^{-w^2} \to 0$. Thus the first summand on the right-hand side vanishes. For the second summand we have $1 - e^{-w} \to 1$ and $y^{(\lceil\alpha\rceil)}(\xi_2) \to y^{(\lceil\alpha\rceil)}(x)$ because $\xi_2 \in [x - w^{-1}, x]$. Thus, we conclude

$$\lim_{w\to\infty} w^2 \int_0^x y^{(\lceil\alpha\rceil)}(\tau) e^{-(x-\tau)w^2}\, d\tau = y^{(\lceil\alpha\rceil)}(x).$$

Inserting this relation into the definition of ϕ, we arrive at

$$\phi(w, x) = (-1)^{\lfloor\alpha\rfloor} \frac{2 \sin \pi\alpha}{\pi} w^{2\alpha - 2\lceil\alpha\rceil - 1} \left[y^{(\lceil\alpha\rceil)}(x) + o(1) \right] \tag{16}$$

which completes the proof of (b).

Finally, part (c) follows directly from the definition of ϕ, viz., Eq. 3. □

In view of parts (a) and (b) of Theorem 3 and Remark 1, we can identify two reasons why the Laguerre method cannot approximate the integral in Eq. 4 very well. Both aspects are related to the fact that the asymptotic behaviour of the integrand function is not taken into account properly.

Indeed the Laguerre method with $\gamma = 0$ as originally proposed [24] firstly assumes the integrand to be smooth at the origin, and by Theorem 3 (a) this assumption is true for our integrand if and only if the exponent of w in Eq. 13 is an integer, i.e. if $\alpha = k + 1/2$ with some $k \in \mathbb{N}_0$.

There are simple ways to circumvent this problem. For example, Lu and Hanyga [14, Eq. 35] have proposed to split the interval of integration in (4) according to

$$D_*^\alpha y(x) = \int_0^\infty \phi(w, x)\, dw = \int_0^c \phi(w, x)\, dw + \int_c^\infty \phi(w, x)\, dw$$

with some constant $c > 0$. Then they use a Gauss-Jacobi quadrature formula with weight function $w^{2\alpha - 2\lceil\alpha\rceil + 1}$ for the integral over $[0, c]$, whereas the integral over $[c, \infty)$ is handled by a shifted Laguerre formula, preceded by some analytical manipulations meant to improve the decay behaviour of the integrand as $w \to \infty$ and hence to speed up the convergence of the shifted Laguerre method. (The original work [14], like [24], only deals with the case $0 < \alpha < 1$, but the generalization to other values of α is obvious.)

An even simpler approach that we shall follow here is to the replace the standard Laguerre formula on $[0, \infty)$, i.e. a Gaussian rule for this interval with weight function e^{-w}, by its generalized version with weight function $w^{2\alpha - 2\lceil\alpha\rceil + 1} e^{-w}$. In other words we choose $\gamma = 2\alpha - 2\lceil\alpha\rceil + 1$ instead of $\gamma = 0$. It is immediately evident that this definition leads to $-1 < \gamma < 1$. In this way we are able to reproduce the correct asymptotic behaviour of the integrand at the origin, thus removing the problem there that slowed down the convergence.

The second, and much more unpleasant, problem is the asymptotic behaviour of the integrand $\phi(w, x)$ as $w \to \infty$ for fixed x. As shown in Theorem 3 (b), the integrand behaves as $w^{2\alpha-2\lceil\alpha\rceil-1}$. The exponent of w here is always contained in the interval $(-3, -1)$. This is just about fast enough to make sure that the improper integral exists, but, no matter how we choose γ, it is far too slow to allow a proper approximation by expressions of the form $w^\gamma e^{-w} p(w)$ with some polynomial p which is what the Laguerre formula attempts. In contrast to the problem at $w = 0$ that we had handled above, there is no easy way to remove this difficulty. Therefore we shall momentarily refrain from introducing additional modifications for the Gauss-Laguerre method. Instead we will summarize the consequences of the findings described so far on the quadrature error:

Theorem 4 *Let $\gamma = 2\alpha - 2\lceil\alpha\rceil + 1$, and assume that $y \in C^{\lceil\alpha\rceil}[0, X]$. Then, the quadrature error for our approximation procedure satisfies the inequality*

$$R_n^{\mathrm{GL}\gamma}\left[(\cdot)^{-\gamma}\exp(\cdot)\phi(\cdot, x)\right] = O\left(n^{\gamma-1}\right)$$

for $x \in [0, X]$.

By definition, $\gamma \in (-1, 1)$, and hence it is clear that the convergence of the Gauss-Laguerre method for this integrand is rather slow.

Proof Our technique of proof is loosely related to the ideas used in [2]. We begin by recalling a property of the Gauss-Laguerre nodes; specifically we have

$$z_{nn}^{(\gamma)} \sim n, \tag{17}$$

see [22, eq. (6.32.4)]. Moreover we use, for fixed x, the auxiliary functions

$$\Phi(w) := w^{-\gamma} e^w \phi(w, x)$$

and

$$\delta_n(w) := \begin{cases} 1 & \text{for } 0 < w \le z_{nn}^{(\gamma)}, \\ 0 & \text{for } 2z_{nn}^{(\gamma)} \le w. \end{cases}$$

On the remaining interval $\left(z_{nn}^{(\gamma)}, 2z_{nn}^{(\gamma)}\right)$ we demand that $0 < \delta_n(w) < 1$ and that $\delta_n \in C^\infty(0, \infty)$. It is well known that such a function exists [2]. Finally we set

$$\Psi_n(w) := \Phi(w)\delta_n(w).$$

It then turns out that

$$R_n^{\mathrm{GL}\gamma}\left[(\cdot)^{-\gamma}\exp(\cdot)\phi(\cdot, x)\right] = R_n^{\mathrm{GL}\gamma}[\Phi] = R_n^{\mathrm{GL}\gamma}[\Phi - \Psi_n] + R_n^{\mathrm{GL}\gamma}[\Psi_n].$$

Since $\Phi(w) = \Psi_n(w)$ for $0 \le x \le z_{nn}^{(\gamma)}$, we conclude $Q_n^{\mathrm{GL}\gamma}[\Phi - \Psi_n] = 0$ and thus

$$\begin{aligned} R_n^{\mathrm{GL}\gamma}[\Phi - \Psi_n] &= \int_0^\infty w^\gamma e^{-w}(\Phi(w) - \Psi_n(w))\,dw \\ &= \int_{z_{nn}^{(\gamma)}}^\infty w^\gamma e^{-w}(\Phi(w) - \Psi_n(w))\,dw \\ &= \int_{z_{nn}^{(\gamma)}}^{2z_{nn}^{(\gamma)}} w^\gamma e^{-w}\Phi(w)(1 - \delta_n(w))\,dw + \int_{2z_{nn}^{(\gamma)}}^\infty w^\gamma e^{-w}\Phi(w)\,dw. \\ &= \int_{z_{nn}^{(\gamma)}}^{2z_{nn}^{(\gamma)}} \phi(w,x)(1 - \delta_n(w))\,dw + \int_{2z_{nn}^{(\gamma)}}^\infty \phi(w,x)\,dw. \end{aligned}$$

Because of Eq. 17 and Theorem 3 (b) we are able to bound the absolute values of these two integrals according to

$$\begin{aligned} &\left| \int_{z_{nn}^{(\gamma)}}^{2z_{nn}^{(\gamma)}} \phi(w,x)(1 - \delta_n(w))\,dw \right| \\ &\quad \le z_{nn}^{(\gamma)} \max_{w \in \left[z_{nn}^{(\gamma)}, 2z_{nn}^{(\gamma)}\right]} |\phi(w,x)| \\ &\quad = O\left(\left(z_{nn}^{(\gamma)}\right)^{2\alpha - 2\lceil\alpha\rceil}\right) = O\left(\left(z_{nn}^{(\gamma)}\right)^{\gamma-1}\right) = O(n^{\gamma-1}) \end{aligned}$$

and

$$\int_{2z_{nn}^{(\gamma)}}^\infty \phi(w,x)\,dw = O\left(\int_{2z_{nn}^{(\gamma)}}^\infty w^{\gamma-2}\,dw\right) = O\left(\left(z_{nn}^{(\gamma)}\right)^{\gamma-1}\right) = O(n^{\gamma-1}),$$

respectively. Thus,

$$R_n^{\mathrm{GL}\gamma}[\Phi - \Psi_n] = O\left(n^{\gamma-1}\right).$$

Moreover, by construction we have that $\Psi_n(w) = 0$ for $w \ge 2z_{nn}^{(\gamma)}$ and $\psi_n \in C^\infty(0,\infty)$. This allows us to invoke [2, Corollary 2.1] to conclude that

$$R_n^{\mathrm{GL}\gamma}[\Psi_n] = O(n^{\gamma-1})$$

too, which completes the proof. □

3.2 The contribution of the ODE solver

The second part of the overall error of the method comes in because of the fact that the differential equation (5) is not solved exactly. However, according to Eq. 10, it is not the error E_h of the differential equation solver itself as defined in (12) but the Gauss-Laguerre quadrature applied to the product of E_h and the reciprocal of the generalized Laguerre weight function, viz. the quantity $Q_n^{\mathrm{GL}\gamma}[(\cdot)^{-\gamma}\exp(\cdot)E_h(\cdot,x)]$, that we need to estimate. Nevertheless it is useful to look at E_h first.

Recall that the differential equation (5) needs to be solved for $w = z_{kn}^{(\gamma)}$, $k = 1, 2, \ldots, n$. The potential problem here is that the absolute value of the

coefficient of ϕ on the right-hand side of the differential equation, viz. the number w^2, grows as $n \to \infty$ at least for some values of k. For example, in the case $k = n$ we have $z_{kn}^{(\gamma)} \sim n$, and hence $w^2 \sim n^2$. To be more precise $z_{kn}^{(\gamma)}$ is slightly less than $4n + 2\gamma + 2$, see [22, eq. (6.32.4)], and hence the value of w^2 can go up to 400 already for $n = 5$, or up to 6400 for $n = 20$. But it is well known [13, Chapter IV] that explicit one-step methods for ordinary differential equations are likely to fail under such conditions because of their insufficient stability properties unless the step sizes are chosen extremely small. Many implicit methods, on the other hand, do not share this unpleasant feature, and thus they can be employed in our situation with a much larger step size. For this reason we shall exclusively work with A-stable implicit methods. For the sake of simplicity we shall also restrict our attention to one-step methods. We shall denote the convergence order of our method by p.

The usual convergence proofs for a numerical method applied to the generic differential equation

$$u'(x) = f(x, u(x))$$

require the step size h to satisfy the condition $hL < 1$, where L is the Lipschitz constant of f with respect to the second variable. In our case, viz. the differential equation (5), we have $L = w^2$, and since we have to solve this equation for $w = z_{kn}^{(\gamma)}$, $k = 1, 2, \ldots, n$, we shall always assume that

$$h < \left(z_{nn}^{(\gamma)}\right)^{-2} \sim n^{-2}. \tag{18}$$

Our first result is then

Lemma 1 *Under the assumptions above, there exists a constant $C > 0$ such that*

$$\left|E_h\left(z_{kn}^{(\gamma)}, x\right)\right| \le Ch^p \exp\left(3\left(z_{kn}^{(\gamma)}\right)^2 X\right)$$

for $k = 1, 2, \ldots, n$, sufficiently small $h > 0$, and $x \in [0, X]$.

Proof The standard error estimate for implicit one-step methods reads, in our notation,

$$\left|E_h\left(z_{kn}^{(\gamma)}, x\right)\right| \le \frac{D}{hK(1 - hL)} e^{KX}$$

(see, e.g., [20, Thm. 9.2]). Here L is the Lipschitz constant of the right-hand side, i.e. $L = \left(z_{kn}^{(\gamma)}\right)^2$, and D is the local discretization error which is bounded by $O(Lh^{p+1})$, while $K = 2L/(1 - hL)$. Combining all these relations we obtain

$$\left|E_h\left(z_{kn}^{(\gamma)}, x\right)\right| = O\left(h^p \exp \frac{2\left(z_{kn}^{(\gamma)}\right)^2 X}{1 - h\left(z_{kn}^{(\gamma)}\right)^2}\right).$$

If h is sufficiently small then the denominator of the argument of the exponential function is greater than 2/3 which implies the claim. □

Based on this result we can estimate the entire contribution due to the differential equation solver:

Theorem 5 *Under the assumptions of Lemma* 1*, there exists a constant* $C > 0$ *such that*

$$\left|Q_n^{\mathrm{GL}\gamma}\left[(\cdot)^{-\gamma}\exp(\cdot)E_h(\cdot,x)\right]\right| \le Ch^p\int_0^{4n}\exp\left(3Xz^2\right)dz.$$

Proof Evidently,

$$Q_n^{\mathrm{GL}\gamma}\left[(\cdot)^{-\gamma}\exp(\cdot)E_h(\cdot,x)\right] = \sum_{k=1}^{n} w_{kn}^{(\gamma)}\left(z_{kn}^{(\gamma)}\right)^{-\gamma} e^{z_{kn}^{(\gamma)}} E_h\left(z_{kn}^{(\gamma)},x\right).$$

For the first summand we use Lemma 1 and the facts that $z_{1n}^{(\gamma)} \sim n^{-1}$ and $w_{1n}^{(\gamma)} \sim n^{-1-\gamma}$ (see, e.g., [2, § 2]) to estimate

$$\left|w_{1n}^{(\gamma)}\left(z_{1n}^{(\gamma)}\right)^{-\gamma} e^{z_{1n}^{(\gamma)}} E_h\left(z_{1n}^{(\gamma)},x\right)\right| = O(h^p)n^{-1}\exp\left(\frac{1}{n}+\frac{3X}{n^2}\right) = O(n^{-1}h^p).$$

For the remaining summands we use Lemma 1 and the identity

$$w_{kn}^{(\gamma)}\left(z_{kn}^{(\gamma)}\right)^{-\gamma} e^{z_{kn}^{(\gamma)}} \sim z_{kn}^{(\gamma)} - z_{k-1,n}^{(\gamma)}$$

which holds for $k = 2, 3, \ldots, n$ [2, eq. (2.3)] to derive

$$\begin{aligned}&\left|Q_n^{\mathrm{GL}\gamma}\left[(\cdot)^{-\gamma}\exp(\cdot)E_h(\cdot,x)\right]\right| \\ &\quad\le O(h^p)\left(n^{-1}+\sum_{k=2}^{n}\left(z_{kn}^{(\gamma)}-z_{k-1,n}^{(\gamma)}\right)\exp\left(3\left(z_{kn}^{(\gamma)}\right)^2 X\right)\right).\end{aligned}$$

The sum on the right-hand side of this inequality is a Riemann sum for the integral $\int_{z_{1n}^{(\gamma)}}^{z_{nn}^{(\gamma)}}\exp(3Xz^2)dz$ which, together with the fact that $z_{nn}^{(\gamma)} = 4n(1+o(1))$ (see above) completes the proof. □

3.3 Summary of the error analysis

Formally, we obtain the following immediate consequence of Theorems 4 and 5:

Theorem 6 *Let* $\gamma = 2\alpha - 2\lceil\alpha\rceil + 1$*, and assume that* $y \in C^{\lceil\alpha\rceil}[0, X]$*. If the ordinary differential equation solver is an A-stable implicit method of order* p *with step size* $h < \left(z_{nn}^{(\gamma)}\right)^{-2}$ *then the error for our approximation procedure satisfies the inequality*

$$\left|R_{n,h}^{\alpha}y(x)\right| = O\left(n^{\gamma-1}\right) + O(h^p)\int_0^{4n}\exp\left(3Xz^2\right)dz$$

for $x \in [0, X]$.

A typical way to proceed would be to choose the number n of integration points first and then to select h such that the second part of the error as given in Theorem 6 roughly is of the same magnitude as the first part. However, our numerical experiments (see Section 6) indicate that the implied constant in the second O-term is much smaller than that of the first. Thus, we have reason to believe that the first term will usually dominate the entire error, and therefore it will not be necessary to use excessively small stepsizes in the differential equation solver. Indeed it is often not even necessary to satisfy the restriction $h < \left(z_{nn}^{(\gamma)}\right)^{-2}$, see our first example in Section 6 and, in particular, Fig. 1.

Summing up our findings on the overall error of the Yuan-Agrawal method, we find that the error due to the differential equation solver will be rather well behaved and unproblematic, at least if an algorithm with sufficiently good stability properties is chosen. The quadrature part of the approach is much less nice, and it is this contribution that is responsible for the major share of the error.

3.4 Results for Chatterjee's variant of the method

As indicated at the end of Section 2, the results developed above can also be transferred to Chatterjee's variant of the algorithm. In this context we find an analogue of Theorem 3:

Theorem 7 *Let $x \in (0, X)$ be fixed and $0 < \alpha \notin \mathbb{N}$, and assume that there exists some $C > 0$ such that $|y^{(\lceil\alpha\rceil)}(\tilde{x})| > C$ for all $\tilde{x} \in [0, X]$.*

(a) *The function $\phi^*(\cdot, x)$ described in Eq. 7 behaves as*

$$\phi^*(w, x) \sim 1 \quad \text{as } w \to 0. \tag{19}$$

(b) *Moreover,*

$$\phi^*(w, x) \sim w^{-1/(\alpha-\lceil\alpha\rceil+1)} \quad \text{as } w \to \infty. \tag{20}$$

(c) *We have $\phi^*(\cdot, x) \in C^\infty(0, \infty)$.*

The proof proceeds along the same lines as the proof of Theorem 3.

It is of interest here to look at the exponent of w on the right-hand side of Eq. 20. To this end, let $\alpha = K + \epsilon$ with some $K \in \mathbb{N}_0$ and $0 < \epsilon < 1$. Then, the exponent in question is $-1/\epsilon$. This is always less than -1, and hence the improper integral converges. In the original Yuan-Agrawal method the exponent could not be smaller than -3; no such bound exists in Chatterjee's approach. In particular, if ϵ is close to 0 then the exponent may be arbitrarily large in modulus, leading to a much faster (but still algebraic) decay of the integrand.

4 A first improvement of the method

In view of the unsatisfactory convergence behaviour of the Gauss-Laguerre formulas demonstrated in Section 3.1, it is of interest to replace them by some other method that is more promising for integrands with an algebraic decay. We shall introduce a suitable candidate in Section 4.1 and discuss the implications of this modification on the differential equation solver in Section 4.2.

4.1 An alternative quadrature rule

Our choice of a candidate for such a better algorithm is motivated by the development of Gautschi [11, § 3]. The idea is to rewrite the integral in Eq. 4 in the form

$$\int_0^\infty \phi(w,x)\,dw = \int_{-1}^{1} (1-t)^{\bar\alpha}(1+t)^{-\bar\alpha}\bar\phi(t,x)\,dt \tag{21}$$

with

$$\bar\alpha := 2\alpha - 2\lceil\alpha\rceil + 1 \in (-1,1) \tag{22}$$

and

$$\bar\phi(t,x) := 2(1-t)^{-\bar\alpha}(1+t)^{\bar\alpha-2}\phi\left(\frac{1-t}{1+t},x\right). \tag{23}$$

The derivation of Eq. 21 follows from the definitions (23) and (22) of $\bar\phi$ and $\bar\alpha$, respectively, using the substitution of variables

$$t = \frac{1-w}{1+w}, \qquad w = \frac{1-t}{1+t}$$

and some straightforward calculations. For our purposes it is useful to note some of the basic properties of the function $\bar\phi$ that correspond to the properties of ϕ described in Theorem 3:

Theorem 8 *Let $x \in (0, X)$ be fixed and $0 < \alpha \notin \mathbb{N}$, and assume that there exists some $C > 0$ such that $|y^{(\lceil\alpha\rceil)}(\tilde x)| > C$ for all $\tilde x \in [0, X]$.*

(a) *The function $\bar\phi(\cdot, x)$ defined in Eq. 23 satisfies*

$$\lim_{t\to 1-} \bar\phi(t,x) = (-1)^{\lfloor\alpha\rfloor} 2^{2\alpha-2\lceil\alpha\rceil+1} \frac{\sin\pi\alpha}{\pi}\left(y^{(\lceil\alpha\rceil-1)}(x) - y^{(\lceil\alpha\rceil-1)}(0)\right). \tag{24}$$

(b) *Moreover,*

$$\lim_{t\to -1+} \bar\phi(t,x) = (-1)^{\lfloor\alpha\rfloor} 2^{1-2\alpha+2\lceil\alpha\rceil} \frac{\sin\pi\alpha}{\pi} y^{(\lceil\alpha\rceil)}(x). \tag{25}$$

(c) *We have $\bar\phi(\cdot, x) \in C^\infty[-1, 1]$.*

Notice that, under our assumptions, the expressions on the right-hand sides of Eqs. 24 and 25 are finite non-zero numbers.

Proof Statements (a) and (b) are immediate consequences of Eqs. 22 and 23 in combination with Eqs. 15 and 16, respectively.

The fact that $\bar{\phi}(\cdot, x)$ has infinitely many derivatives inside the open interval $(-1, 1)$ follows from Eq. 23 and Theorem 3 (c). Thus, to complete the proof of (c) it remains to show that the one-sided limits

$$\lim_{t\to 1-} \frac{\partial^\ell}{\partial t^\ell}\bar{\phi}(t, x) \quad \text{and} \quad \lim_{t\to -1+} \frac{\partial^\ell}{\partial t^\ell}\bar{\phi}(t, x)$$

exist for all $\ell \in \mathbb{N}$. To this end we combine Eqs. 23 and 3 and find

$$\bar{\phi}(t, x) = (-1)^{\lfloor\alpha\rfloor} \frac{4 \sin \pi\alpha}{\pi} (1 + t)^{-2} \int_0^x y^{(\lceil\alpha\rceil)}(\tau) \exp\left(-(x - \tau)\left(\frac{1 - t}{1 + t}\right)^2\right) d\tau.$$

From this representation it is immediately evident that all derivatives at $t = 1$ exist. At $t = -1$ we will not encounter any differentiability problems either because the negative powers of $(1 + t)$ that arise in higher-order derivatives of $\bar{\phi}$ will always be cancelled by the exponential function whose argument behaves as $-c(1 + t)^{-2}$ as $t \to -1$ with some $c > 0$ which implies that the exponential always decays faster than the algebraic term grows. □

Bearing in mind the information on $\bar{\phi}$ provided in Theorem 8, it is a natural idea to approximate the integral on the right-hand side of Eq. 21 by a Gauss-Jacobi quadrature rule with respect to the weight function $(1 - t)^{\bar{\alpha}}(1 + t)^{-\bar{\alpha}}$ as suggested in [11, § 3]. Thus, instead of the method mentioned in Eq. 9, we suggest to use the formula

$$\bar{D}^\alpha_{n,h} y(x) := 2 \sum_{k=1}^{n} W^{(\bar{\alpha})}_{kn} \left(1 - Z^{(\bar{\alpha})}_{kn}\right)^{-\bar{\alpha}} \left(1 + Z^{(\bar{\alpha})}_{kn}\right)^{\bar{\alpha}-2} \phi_h\left(\frac{1 - Z^{(\bar{\alpha})}_{kn}}{1 + Z^{(\bar{\alpha})}_{kn}}, x\right), \quad (26)$$

where $W^{(\bar{\alpha})}_{kn}$ and $Z^{(\bar{\alpha})}_{kn}$ are the weights and nodes, respectively, of the Gauss-Jacobi quadrature formula for the weight function $(1 - t)^{\bar{\alpha}}(1 + t)^{-\bar{\alpha}}$. We may then expect a much more rapid convergence of the quadrature than in the original algorithm analyzed in Section 3.1. To be precise, in view of Theorem 8 we find the following result which obviously is a strong improvement over Theorem 4:

Theorem 9 *Let $\bar{\alpha} = 2\alpha - 2\lceil\alpha\rceil + 1$, and assume that $y \in C^{\lceil\alpha\rceil}[0, X]$. Then, for every $\ell \in \mathbb{N}$ the quadrature error for our approximation procedure satisfies the inequality*

$$R^{\mathrm{GJ}\bar{\alpha}}_n \left[\bar{\phi}(\cdot, x)\right] = O\left(n^{-\ell}\right)$$

for $x \in [0, X]$.

Proof Let $\ell \in \mathbb{N}$. We know by Theorem 8 that the integrand $\bar{\phi}$ is ℓ times continuously differentiable on $[-1, 1]$. Thus the quadrature error can be bounded by $O(n^{-\ell})$ as required [6]. □

4.2 Implications on the differential equation solver

Notice that according to [22, Thm. 8.1.2] the smallest node of the Gauss-Jacobi method behaves as $-1+cn^{-2}$ for $n\to\infty$. Because of the transformation of variables underlying our method, this means that the largest point at which our quadrature method evaluates the function ϕ is located at $cn^2(1+o(1))$ with some $c>0$. This is even larger than the corresponding point in the Gauss-Laguerre method used in the original Yuan-Agrawal scheme where we only had a value of cn, see Section 3.2. Three consequences of this observation need to be noted: First of all, the value of $\phi(w,x)$ is taken into account for much larger values of w which, in view of the slow decay of $\phi(w,x)$ as $w\to\infty$ observed in Theorem 3 (b), is a main reason for the superiority of the Gauss-Jacobi method. Second, explicit methods for the solution of the ordinary differential equations are even less useful unless extremely small stepsizes are chosen. And finally, we find a direct analogue of Lemma 1:

Lemma 2 *If E_h is the error of an A-stable implicit differential equation solver with step size $h<\left(1+Z_{1n}^{(\bar\alpha)}\right)^2\left(1-Z_{1n}^{(\bar\alpha)}\right)^{-2}\sim n^{-4}$, then there exists a constant $C>0$ such that*

$$\left|E_h\left(\left(1-Z_{kn}^{(\bar\alpha)}\right)\Big/\left(1+Z_{kn}^{(\bar\alpha)}\right),x\right)\right|\le Ch^p\exp\left(3\left(\frac{1-Z_{kn}^{(\bar\alpha)}}{1+Z_{kn}^{(\bar\alpha)}}\right)^2X\right)$$

The proof of this result is completely analoguous to the proof of Lemma 1. From Lemma 2 we then conclude:

Theorem 10 *Under the assumptions of Lemma 2, there exists a constant $C>0$ such that*

$$\left|Q_n^{\mathrm{GJ}\bar\alpha}[(1-\cdot)^{-\bar\alpha}(1+\cdot)^{\bar\alpha-2}E_h((1-\cdot)/(1+\cdot),x)]\right|\le Ch^p\int_0^n z\exp\left(\frac{48}{\pi}Xz^4\right)dz.$$

Proof In view of Lemma 2 we have

$$\begin{aligned}&\left|Q_n^{\mathrm{GJ}\bar\alpha}\left[(1-\cdot)^{-\bar\alpha}(1+\cdot)^{\bar\alpha-2}E_h((1-\cdot)/(1+\cdot),x)\right]\right|\\&\quad\le Ch^p\sum_{k=1}^n W_{kn}^{(\bar\alpha)}\left(1-Z_{kn}^{(\bar\alpha)}\right)^{-\bar\alpha}\left(1+Z_{kn}^{(\bar\alpha)}\right)^{\bar\alpha-2}\exp\left(3\left(\frac{1-Z_{kn}^{(\bar\alpha)}}{1+Z_{kn}^{(\bar\alpha)}}\right)^2X\right).\end{aligned}$$

Let $\epsilon\in(0,1)$ be fixed. Then, from [5] we recall the relations

$$W_{kn}^{(\bar\alpha)}\left(1-Z_{kn}^{(\bar\alpha)}\right)^{-\bar\alpha}\left(1+Z_{kn}^{(\bar\alpha)}\right)^{\bar\alpha}\sim\begin{cases}\pi n^{-1}\left(1-\left(Z_{kn}^{(\bar\alpha)}\right)^2\right)^{1/2} & \text{for all } k,\\ \frac{1}{2}\left|Z_{k+1,n}^{(\bar\alpha)}-Z_{k-1,n}^{(\bar\alpha)}\right| & \text{for all } k \text{ such that } Z_{kn}^{(\bar\alpha)}\in[-1+\epsilon,1-\epsilon].\end{cases}$$

These relations suggest that we decompose the sum above into three parts S_1, S_2 and S_3, the first of which contains the summands where k is such that $Z_{kn}^{(\tilde{\alpha})} \in [-1+\epsilon, 1-\epsilon]$ whereas the second part consists of the summands with $Z_{kn}^{(\tilde{\alpha})} \in (1-\epsilon, 1)$ and the third one contains the remaining summands. Then we may combine our formulas above to conclude

$$S_1 \le \frac{1}{2} \sum_{Z_{kn}^{(\tilde{\alpha})} \in [-1+\epsilon, 1-\epsilon]} \left| Z_{k+1,n}^{(\tilde{\alpha})} - Z_{k-1,n}^{(\tilde{\alpha})} \right| \left(1+Z_{kn}^{(\tilde{\alpha})}\right)^{-2} \exp\left(3X\left(1-Z_{kn}^{(\tilde{\alpha})}\right)^2 \left(1+Z_{kn}^{(\tilde{\alpha})}\right)^{-2}\right)$$

which is a Riemann sum for the integral

$$\frac{1}{2}\int_{1-\epsilon}^{1+\epsilon} (1-z)^{-2} \exp(3X(1-z)^2(1+z)^{-2})dz,$$

a constant. Thus $S_1 = O(1)$. To estimate S_2 we write

$$S_2 = O(n^{-1}) \sum_{Z_{kn}^{(\tilde{\alpha})} \in [1-\epsilon, 1]} \left(1-\left(Z_{kn}^{(\tilde{\alpha})}\right)^2\right)^{1/2} \left(1+Z_{kn}^{(\tilde{\alpha})}\right)^{-2} \exp\left(3X\left(\frac{1-Z_{kn}^{(\tilde{\alpha})}}{1+Z_{kn}^{(\tilde{\alpha})}}\right)^2\right)$$

$$\le \epsilon^{-2} \exp(3X(2-\epsilon)^2\epsilon^{-2})\, O(n^{-1}) \sum_{Z_{kn}^{(\tilde{\alpha})} \in [1-\epsilon, 1]} \left(1-\left(Z_{kn}^{(\tilde{\alpha})}\right)^2\right)^{1/2}$$

and introduce the trigonometric representation of the Gauss-Jacobi nodes, viz. $Z_{kn}^{(\tilde{\alpha})} = \cos\theta_{kn}$. From [22, Thm. 8.9.1] we know that $\theta_{kn} = (k\pi + O(1))/n$, and hence we may continue the estimation of S_2 via

$$S_2 = O(n^{-1}) \sum_{\theta_{kn} \in [0, \arccos(1-\epsilon)]} \sin\theta_{kn} = O(n^{-2}) \sum_{k=1}^{\lceil n \arccos(1-\epsilon)\rceil} (k + O(1)) = O(1).$$

Finally, we need to look at S_3. Here again we shall use the trigonometric representation and the facts that

$$\left(1+Z_{kn}^{(\tilde{\alpha})}\right)^{-2} = \left(\frac{1-\left(Z_{kn}^{(\tilde{\alpha})}\right)^2}{1-Z_{kn}^{(\tilde{\alpha})}}\right)^{-2} = \frac{\left(1-Z_{kn}^{(\tilde{\alpha})}\right)^2}{\sin^4\theta_{kn}} \le \frac{4}{\sin^4\theta_{kn}}$$

and (as an immediate consequence)

$$\left(\frac{1-Z_{kn}^{(\tilde{\alpha})}}{1+Z_{kn}^{(\tilde{\alpha})}}\right)^2 \le 4\left(1+Z_{kn}^{(\tilde{\alpha})}\right)^{-2} \le \frac{16}{\sin^4\theta_{kn}}$$

to conclude

$$
\begin{aligned}
S_3 &= \sum_{Z_{kn}^{(\bar\alpha)}\in(-1,-1+\epsilon)} W_{kn}^{(\bar\alpha)}\left(1-Z_{kn}^{(\bar\alpha)}\right)^{-\bar\alpha}\left(1+Z_{kn}^{(\bar\alpha)}\right)^{\bar\alpha-2}\exp\left(3\left(\frac{1-Z_{kn}^{(\bar\alpha)}}{1+Z_{kn}^{(\bar\alpha)}}\right)^2 X\right)\\
&\le O\left(n^{-1}\right)\sum_{Z_{kn}^{(\bar\alpha)}\in(-1,-1+\epsilon)}\left(1+Z_{kn}^{(\bar\alpha)}\right)^{-2}\sin\theta_{kn}\exp\left(3\left(\frac{1-Z_{kn}^{(\bar\alpha)}}{1+Z_{kn}^{(\bar\alpha)}}\right)^2 X\right)\\
&\le O(n^{-1})\sum_{\theta_{kn}\in[\arccos(-1+\epsilon),\pi]}(\sin\theta_{kn})^{-3}\exp\left(48X(\sin\theta_{kn})^{-4}\right)\\
&\le O(n^2)\sum_{k=1}^{\lceil n\arccos(1-\epsilon)\rceil}k^{-3}\exp\left(\frac{48}{\pi}Xn^4k^{-4}\right).
\end{aligned}
$$

The rightmost sum is a Riemann sum for the integral

$$
\begin{aligned}
&\int_1^{\lceil n\arccos(1-\epsilon)\rceil+1} z^{-3}\exp\left(\frac{48}{\pi}Xn^4z^{-4}\right)dz\\
&\quad=\int_{n/(\lceil n\arccos(1-\epsilon)\rceil+1)}^{n}\frac{u}{n^2}\exp\left(\frac{48}{\pi}Xu^4\right)du\le n^{-2}\int_0^n u\exp\left(\frac{48}{\pi}Xu^4\right)du,
\end{aligned}
$$

and thus the claim follows. □

4.3 Summary

In analogy with Theorem 6 we can summarize the error analysis for our modified algorithm as follows:

Theorem 11 *Let $\bar\alpha = 2\alpha - 2\lceil\alpha\rceil + 1$, and assume that $y \in C^{\lceil\alpha\rceil}[0, X]$. If the ordinary differential equation solver is an A-stable implicit method of order p with step size $h < \left(1+Z_{1n}^{(\bar\alpha)}\right)^2\left(1-Z_{1n}^{(\bar\alpha)}\right)^{-2}$ then the error for our approximation procedure satisfies the inequality*

$$
\left|\bar R_{n,h}^{\alpha}y(x)\right| = O(n^{-\ell}) + O(h^p)\int_0^n z\exp\left(\frac{48}{\pi}Xz^4\right)dz
$$

for every $\ell \in \mathbb{N}$ and for all $x \in [0, X]$.

4.4 Application of the Gauss-Jacobi method to Chatterjee's variant

In view of Theorem 7, we can also apply the theory developed above to Chatterjee's variant of the approach, i.e. for the computation of $D_*^{\alpha}y(x)$ via

Eq. 8. To this end we have to follow Gautschi's path as we had done above for the Yuan-Agrawal method, thus giving

$$\widetilde{D}^{\alpha}_{n,h} y(x) := 2 \sum_{k=1}^{n} V^{(\alpha)}_{kn} \left(1 + Y^{(\alpha)}_{kn}\right)^{-1/(\alpha - \lceil \alpha \rceil + 1)} \phi^{*}_{h} \left(\frac{1 - Y^{(\alpha)}_{kn}}{1 + Y^{(\alpha)}_{kn}}, x \right), \tag{27}$$

where $Y^{(\alpha)}_{kn}$ and $V^{(\alpha)}_{kn}$ are the nodes and weights of the Gauss-Jacobi quadrature on $[-1, 1]$ for the weight function $(1+t)^{-2+1/(\alpha - \lceil \alpha \rceil + 1)}$. Once again, the computation of a numerical solution ϕ^{*}_{h} of the differential equation (6) should be done by an A-stable implicit method.

In Theorem 8 (c) we had seen that the integrand of the transformed integral in the original method, i.e. the function to which the Gauss-Jacobi quadrature is applied, has infinitely many derivatives on the interval $(-1, 1)$ and at both end points of this interval. For the corresponding function in Chatterjee's variant, the property is also easy to see on $(-1, 1)$. At the end points, however, the non-integer nature of the exponent of w in the argument of the exponential function in Eq. 7 implies that we only have continuity but not differentiability. Thus we must expect a weaker performance of the Gauss-Jacobi method. Therefore we shall not pursue this idea in the context of Chatterjee's variant any further. Rather we shall look at a different approach, both for the Yuan-Agrawal method and for Chatterjee's variant, in the next section.

5 An alternative improvement

So far, we have looked at the two numerical parts of the algorithm, i.e. the solution of the ordinary differential equation (5) and the numerical integration of (4), essentially independently of each other. Alternatively, it is possible to use a coupled approach in the spirit of Singh and Chatterjee [21] who have developed it for Chatterjee's variant of the approach. We shall see that a generalization of this idea can be used for the original Yuan-Agrawal representation too.

Specifically, we shall start with an n-dimensional space of functions $U_n \subset C(0, \infty)$ with a basis $\{\varphi_j : j = 1, 2, \ldots, n\}$, and we aim to find an approximation $\widehat{\phi}$ for our integrand function ϕ in U_n. In other words, we have to find suitable coefficients $a_j(x)$, $j = 1, 2, \ldots, n$, for the representation

$$\widehat{\phi}(w, x) := \sum_{j=1}^{n} a_j(x) \varphi_j(w) \approx \phi(w, x). \tag{28}$$

Once we have computed these coefficients, our final approximation for the fractional derivative $D^{\alpha}_{*} y(x)$ will then be

$$\widehat{D}^{\alpha}_{n} y(x) := \int_0^{\infty} \widehat{\phi}(w, x)\, dw = \sum_{j=1}^{n} a_j(x) \int_0^{\infty} \varphi_j(w)\, dw. \tag{29}$$

The computation of the coefficients must be done in such a way that $\widehat{\phi}$ is a sufficiently good approximate solution for the initial value problem (5) or (6). Possible approaches are, e.g., a Galerkin method (this is the proposal of Singh and Chatterjee [21]) or a collocation technique. In both cases the initial condition of Eq. 5 leads to the requirement that

$$0 = \widehat{\phi}(w, 0) = \sum_{j=1}^{n} a_j(0)\varphi_j(w)$$

for all w. In view of the linear independence of the φ_j this implies

$$a_j(0) = 0 \text{ for all } j. \tag{30}$$

The Galerkin approach leads to a system

$$G'a'(x) + Ga(x) = gy^{(\lceil\alpha\rceil)}(x) \tag{31}$$

where $a(x) = (a_1(x), a_2(x), \ldots, a_n(x))^{\mathrm{T}}$, $a'(x) = (a_1'(x), a_2'(x), \ldots, a_n'(x))^{\mathrm{T}}$, and the matrices G' and G have components

$$g'_{jk} = \int_0^\infty \varphi_j(w)\varphi_k(w)\,dw \tag{32}$$

and

$$g_{jk} = \begin{cases} \displaystyle\int_0^\infty w^2\varphi_j(w)\varphi_k(w)\,dw & \text{for the Yuan-Agrawal equation (5),} \\ \displaystyle\int_0^\infty w^{1/(\alpha-\lceil\alpha\rceil-1)}\varphi_j(w)\varphi_k(w)dw & \text{for Chatterjee's variant (6),} \end{cases} \tag{33}$$

respectively, while the components g_j of the vector g are given by

$$g_j = \begin{cases} (-1)^{\lfloor\alpha\rfloor}\dfrac{2\sin\pi\alpha}{\pi}\displaystyle\int_0^\infty w^{2\alpha-2\lceil\alpha\rceil+1}\varphi_j(w)dw & \text{for Eq. 5,} \\ (-1)^{\lfloor\alpha\rfloor}\dfrac{2\sin\pi\alpha}{\pi(\alpha-\lceil\alpha\rceil+1)}\displaystyle\int_0^\infty \varphi_j(w)dw & \text{for Eq. 6.} \end{cases} \tag{34}$$

Equations 30 and 31 constitute an n-dimensional initial value problem of order 1 with constant coefficients that will typically be solved numerically.

The collocation method for Eq. 5 or 6 means that the coefficients $a_j(x)$ can be found by choosing n collocation points $w_j \in (0, \infty)$, $j = 1, 2, \ldots, n$, and solving the system

$$H'a'(x) + Ha(x) = hy^{(\lceil\alpha\rceil)}(x) \tag{35}$$

where $a(x)$ and $a'(x)$ are as in the Galerkin method, while now the matrices H' and H have components

$$h'_{jk} = \varphi_k(w_j) \tag{36}$$

and

$$h_{jk} = \begin{cases} w_j^2\varphi_k(w_j) & \text{for the Yuan-Agrawal equation (5),} \\ w_j^{1/(\alpha-\lceil\alpha\rceil-1)}\varphi_k(w_j) & \text{for Chatterjee's variant (6),} \end{cases} \tag{37}$$

respectively, while the components h_j of the vector h are given by

$$h_j = \begin{cases} (-1)^{\lfloor\alpha\rfloor} \dfrac{2\sin\pi\alpha}{\pi} w_j^{2\alpha-2\lceil\alpha\rceil+1} & \text{for Eq. 5,} \\ (-1)^{\lfloor\alpha\rfloor} \dfrac{2\sin\pi\alpha}{\pi(\alpha-\lceil\alpha\rceil+1)} & \text{for Eq. 6.} \end{cases} \tag{38}$$

Equations 30 and 35 also constitute an n-dimensional initial value problem of order 1 with constant coefficients that will typically be solved numerically.

In either case, it is advisable to choose the basis functions φ_j (and hence the approximation space U_n) such that the following conditions are satisfied:

1. The explicit computation of the integrals $\int_0^\infty \varphi_j(w)dw$ appearing in Eq. 29 should be reasonably easy.
2. Every φ_j should either vanish identically or reproduce the asymptotic behaviour of $\varphi(w, x)$ as $w \to 0$ and as $w \to \infty$ described in Theorem 3 (for the Yuan-Agrawal method) or Theorem 7 (for Chatterjee's variant).
3. For the Galerkin method we need to make sure that the integrals given in Eqs. 32, 33 and 34 exist, while for the collocation method no such additional condition needs to be imposed.

Of course the error analysis depends heavily on the precise choice of the functions φ_j. Moreover the (numerical or analytical) computation of the entries of the matrices G and G' or H and H', respectively, can be a challenging task. The condition of the coefficient matrices may be a problem for the numerical work too. Therefore we shall defer the analysis of these approaches to a later paper. However, to illustrate the potential of the method, we will present some numerical results in Section 6.

6 Numerical examples

We shall now come to some numerical experiments that will demonstrate the advantage to be expected from our modification.

6.1 Computation of a fractional derivative

We begin by looking at a simple example: Our goal is to compute the fractional derivative $D_*^\alpha y(x)$ for $y(x) = x^3$ and $\alpha = 0.6$ on the interval $x \in [0, 1]$. We first use the original Yuan-Agrawal method, i.e. we approximate the integral in Eq. 4 with an n-point Gauss-Laguerre method. Specifically our experiments were done with $n = 8$, $n = 16$, and $n = 32$. In each case we have solved the first-order differential equations with a trapezoidal method with step sizes $h = 1/10$ and $h = 1/100$, respectively. The resulting absolute errors are shown in Fig. 1 where it can be seen that the differences between the two sets of experiments with identical numbers of quadrature nodes but different step sizes in the differential equation solvers are very small compared to the differences between the results for different numbers of quadrature nodes.

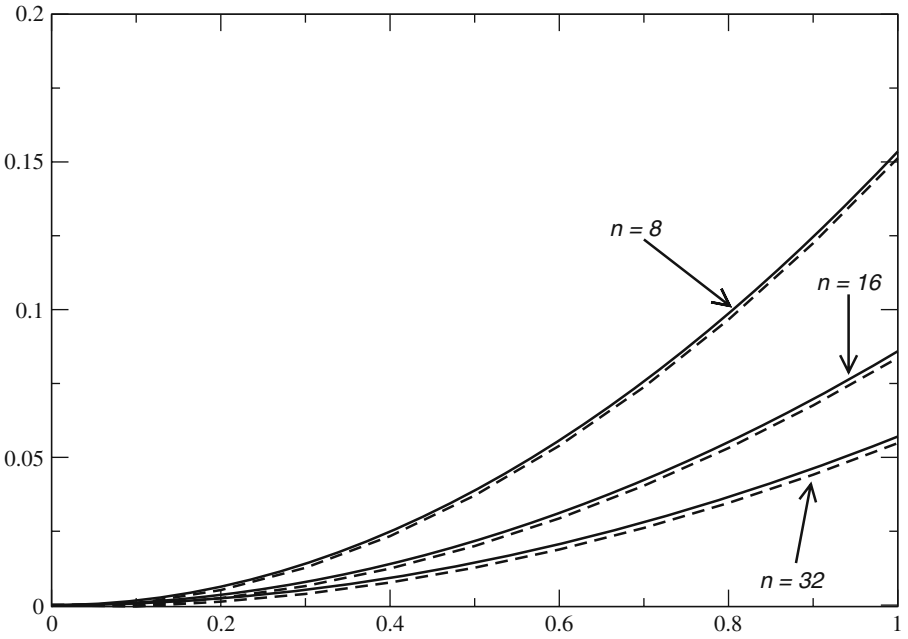

Fig. 1 Absolute errors of the original Yuan-Agrawal method for the approximation of $D_*^{\alpha} y(x)$ with $y(x) = x^3$ for $x \in [0, 1]$, taken with 8, 16 and 32 Gauss-Laguerre nodes and trapezoidal method with $h = 1/10$ (*dashed*) and $h = 1/100$ (*solid lines*)

These examples have then been repeated with our modified algorithm, i.e. with the Gauss-Laguerre method being replaced by a suitably transformed Gauss-Jacobi formula. All other parameters were left unchanged. The results are displayed in Fig. 2. A comparison with Fig. 1 shows some significant differences. First of all, by examining the scales on the vertical axes we note that the magnitude of the error has decreased substantially. The next observation is that it was impossible to distinguish the data for 32 quadrature points from those for 16 nodes graphically, so we only plotted the latter explicitly. Moreover we find that now the quadrature error is so small that the error introduced by the trapezoidal differential equation solver dominates the overall error. Thus, in this sense, the roles of the two parts of the error have been reversed when compared to the original algorithm. All these points clearly reveal that the modification of the quadrature formula indeed results in the theoretically expected performance improvement.

The two quadrature formulas of the original and the modified method, respectively, can both be written in the form

$$\int_0^{\infty} \phi(w, x)\, dw \approx \sum_{k=1}^{n} \rho_{kn} \phi(\sigma_{kn}, x)$$

where the weights ρ_{kn} and the nodes σ_{kn} can be computed from the weights and nodes of the Gauss-Laguerre and Gauss-Jacobi formulas, respectively, by suitable transformations. For $n = 8$ we have plotted the resulting transformed

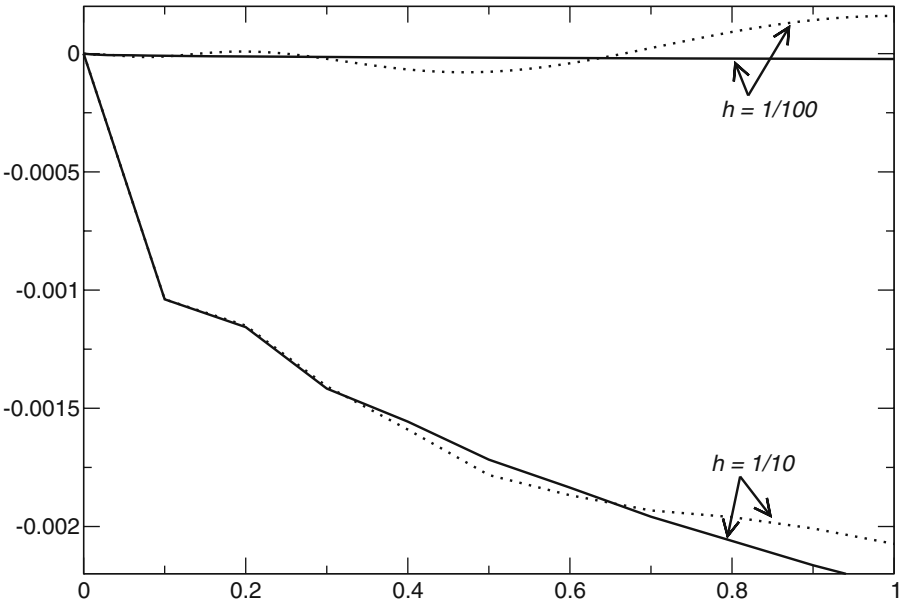

Fig. 2 Absolute errors of the modified Yuan-Agrawal method for the approximation of $D_*^\alpha y(x)$ with $y(x) = x^3$ for $x \in [0, 1]$, taken with 8 (*dotted*) and 16 (*solid lines*) Gauss-Jacobi nodes and trapezoidal method with $h = 1/10$ and $h = 1/100$

pairs of nodes and weights in Fig. 3. It is evident that the nodes for the modified method cover a much larger interval than the original nodes. In view of the slow decay of $\phi(w, x)$ as $w \to \infty$ this explains why the new method works better. We also recall the interpretation of the approach from the mechanical point of view given by Schmidt and Gaul [19] from which it is also apparent that there is a substantial advantage in spreading out the nodes over a larger subinterval of the positive real axis.

For the sake of comparison we have also computed a numerical approximation of the fractional derivative mentioned above by the algorithm discussed in Section 5. Specifically we have used the Galerkin technique described there for the differential equation (5) from the Yuan-Agrawal approach. Our choice of the basis functions φ_j was motivated by the ideas proposed by Singh and Chatterjee [21, §§ 9, 10, and 12]. We use the abbreviation $\gamma := 2\alpha - 2\lceil\alpha\rceil - 1$ and introduce grid points $y_j = 10^{a+(b-a)(j-1)/(n-2)}$ and $p_j := y_j^2/(1+y_j^2)$, $j = 1, 2, \ldots, n-1$, and $p_0 = 0$ and $p_n = 1$ and a transformation of variables $\xi(w) := w^{-\gamma}/(1 + w^{-\gamma})$. Then, our basis functions are

$$\phi_j(w) := \rho(w) h_j(\xi(w)), \qquad j = 1, 2, \ldots, n,$$

where

$$\rho(w) := \begin{cases} w^{\gamma+2}(1 + w^{\gamma+2})^{-1} & \text{if } \gamma > -2, \\ 1 & \text{if } \gamma = -2, \\ 1 + w^{\gamma+2} & \text{if } \gamma < -2, \end{cases}$$

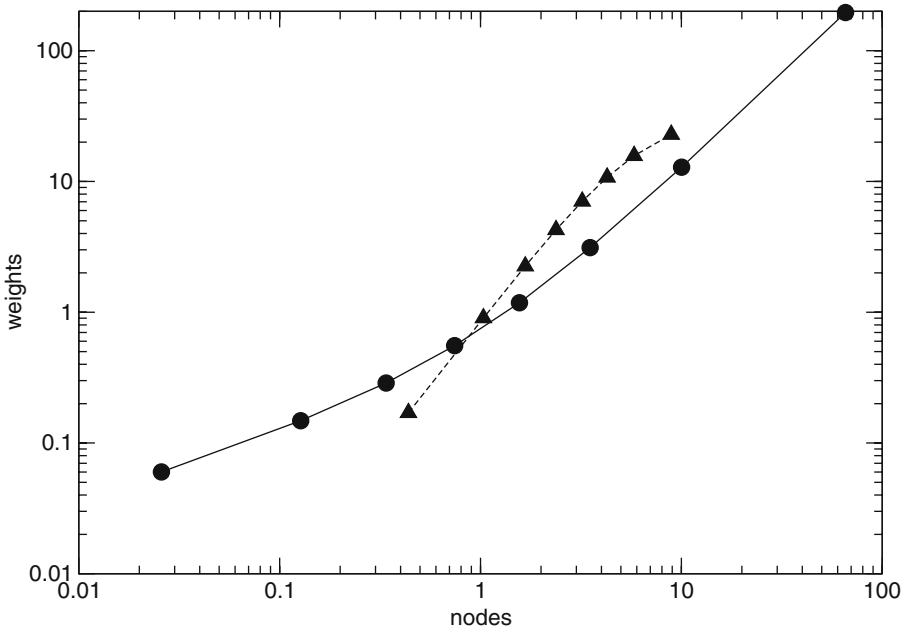

Fig. 3 Log-log plot of transformed quadrature nodes and weights for 8-point Gauss-Laguerre formula in original Yuan-Agrawal method (*triangles*) and for 8-point Gauss-Jacobi formula in modified method (*circles*)

and h_j is the piecewise linear function that takes the value 1 at p_{j-1} and 0 at all $p_k, k \neq j-1$. This choice asserts that the linear combinations of the ϕ_j exhibit the correct asymptotic behaviour for $w \to 0$ and $w \to \infty$ as described in Theorem 3. The absolute errors of our numerical results for the computation of $D_*^{0.6} y(x)$ with $y(x) = x^3$ on [0, 1] using this special case of the method, with parameters $a = -4$ and $b = 3$, are shown in Fig. 4. The differential equation (31) arising in this context has been solved by a trapezoidal method with step sizes $h = 1/10$ and $h = 1/100$, respectively. The data are given for $n = 9$ and $n = 15$. They show that, at least for this choice of basis functions, the results are better than those of the original Yuan-Agrawal method (with a Gauss-Laguerre quadrature) but worse than our modification proposed in Section 4, i.e. the use of the transformed Gauss-Jacobi quadrature. It is possible that better results may be obtained by a different choice of the basis functions, but a systematic investigation of this question is beyond the scope of this paper.

6.2 Solution of a fractional differential equation

Finally we consider an example due to Schmidt and Gaul [19, §§ 2 and 4], the differential equation

$$c D_*^{\alpha} x(t) + k x(t) = f(t), \qquad x(0) = 0, \tag{39}$$

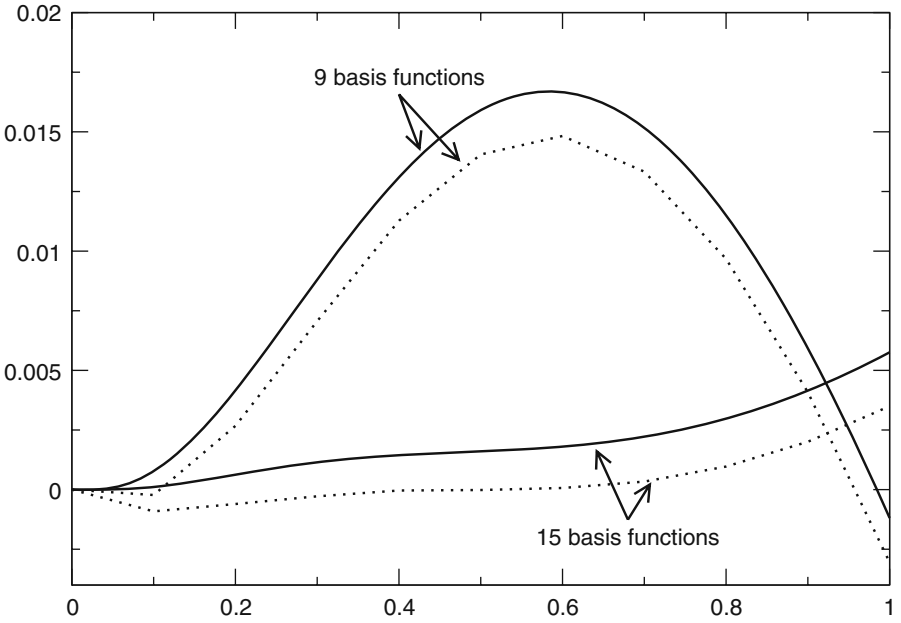

Fig. 4 Absolute errors of the method of Section 5 (Yuan-Agrawal differential equation solved by Galerkin method; resulting differential equation (31) solved by trapezoidal method with step size h) for the approximation of $D_*^\alpha y(x)$ with $y(x) = x^3$ for $x \in [0, 1]$, taken with 9 and 15 basis functions and trapezoidal method with $h = 1/10$ (*dotted*) and $h = 1/100$ (*solid lines*)

with $c = 100$, $k = 10$ and $\alpha = 0.3$. This is the equation of motion of a massless one-dimensional fractional Kelvin-Voigt model subject to the external force $f(t)$ [19, § 2]. We will use the discretization of the variable t by the mesh points

$$t_0 = 0, \quad t_j = t_{j-1} + h_j \qquad (j = 1, 2, \ldots, 5000)$$

with

$$h_1 = 10^{-4} \quad \text{and} \quad h_j = 1.005 h_{j-1} \qquad (j = 2, 3, \ldots, 5000).$$

Thus we cover the interval $t \in [0, 1.35 \cdot 10^9]$. The author has been informed by A. Schmidt (personal communication, 2008) that this was actually the discretization used in the original computations of Schmidt and Gaul [19, § 4]. In order to make the results comparable we have chosen to retain this mesh.

We look at exactly the same situation as Schmidt and Gaul, i.e. we choose

$$f(t) = \begin{cases} 0 & \text{for } t = 0, \\ f_0 & \text{else,} \end{cases} \qquad \text{with } f_0 = 1. \tag{40}$$

The trapezoidal method is used to solve the first-order differential equations arising in the Yuan-Agrawal method. For the numerical integration we have used both the Gauss-Laguerre method proposed by Yuan and Agrawal and the

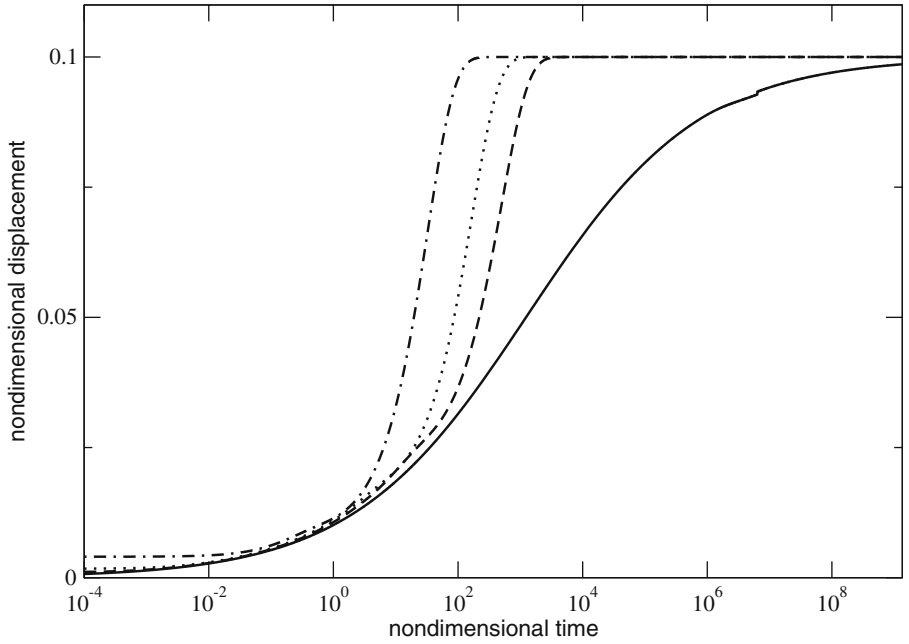

Fig. 5 Exact solution (*solid line*) of Eq. 39 with data given in Eq. 40 and numerical solution with original Yuan-Agrawal method, using trapezoidal ODE solver and 2 (*dash-dotted*), 7 (*dotted*), and 15 (*dashed*) quadrature points, respectively

transformed Gauss-Jacobi method suggested by Gautschi [11] and described in Section 4 with 2, 7, and 15 points, respectively. The results are shown with a logarithmic scale on the horizontal (time) axis in Fig. 5 for the original method and in Fig. 6 for our modified version. The plots show the exact solution,

$$x(t) = \frac{f_0}{k}(1 - E_\alpha(-kt^\alpha/c))$$

(where E_α is the usual Mittag-Leffler function of order α), and the respective numerical results. From a comparison of the two figures, the significant gain in quality obtained by this simple modification (that does not change the computational cost because we have only replaced a quadrature formula with a certain number of nodes by a different one with the same number of nodes) is evident.

In our second experiment we have replaced the trapezoidal method for the solution of the ordinary differential equations in our modified Yuan-Agrawal method by a backward Euler method. This means that we have replaced a second-order by a first-order scheme. Nevertheless it was not possible to distinguish the resulting plots from those obtained by the modified Yuan-Agrawal method with the trapezoidal algorithm as shown in Fig. 6. This emphasizes the fact that the choice of the quadrature routine for the integral is much more

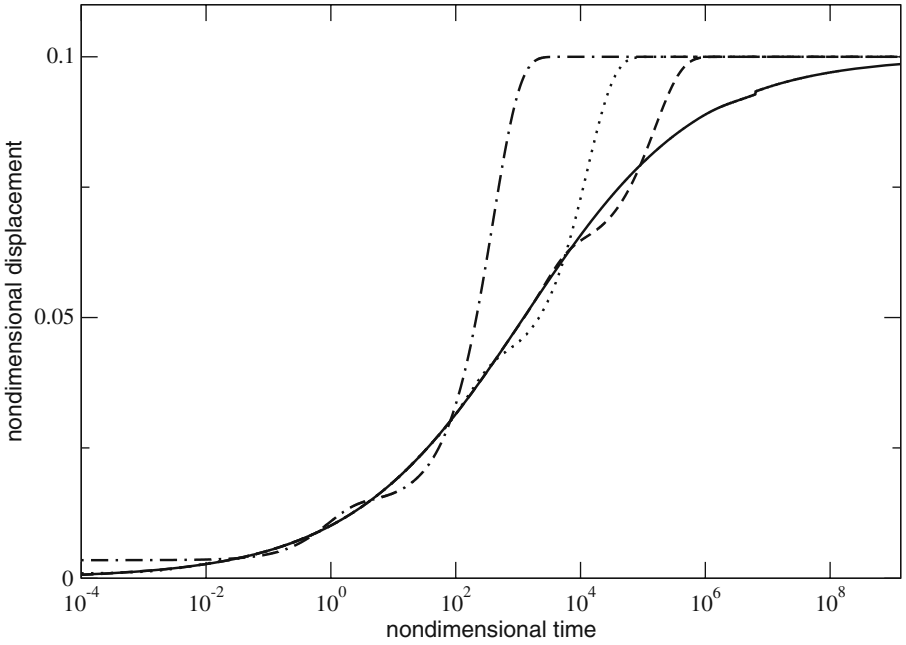

Fig. 6 Exact solution (*solid line*) of Eq. 39 with data given in Eq. 40 and numerical solution with modified method, using trapezoidal ODE solver and 2 (*dash-dotted*), 7 (*dotted*), and 15 (*dashed*) quadrature points, respectively

important than the choice of the differential equation solver, at least as long as the latter is chosen from the class of A-stable implicit methods.

7 Conclusions

The approach of Yuan and Agrawal for the numerical calculation of fractional derivatives of order $\alpha \in (0, 1)$ can be decomposed into three steps:

(a) rewrite the fractional derivative in the form of an integral,
(b) compute the integrand function of this integral by numerically solving a first-order initial value problem,
(c) compute the integral itself numerically using a suitable quadrature formula and the function values of the integrand obtained in step (b).

In our analysis we have first seen that it is possible to extend the approach of Yuan and Agrawal from $0 < \alpha < 1$ to arbitrary positive non-integers α in a straightforward way. This observation refers both to the analytical part of the method, i.e. step (a), and to the numerical part (steps (b) and (c)).

Many options are available when it comes to selecting the solver for the ordinary differential equations required in step (b). Explicit methods seem to be of little practical use, but A-stable implicit schemes can be used according

to the user's personal preferences without having to worry about any potential negative influence on the final result.

The really crucial part of the method is the choice of the quadrature formula in step (c). As observed elsewhere [19], the original proposal of Yuan and Agrawal [24], i.e. the Gauss-Laguerre rule, leads to a very poor quality of the algorithm. We have identified the reason for this unsatisfactory behaviour, it being the asymptotics of the integrand function ϕ. Based on this result we have been able to propose an alternative quadrature formula that gives rise to a much better overall performance of the scheme. We believe that this modified version of the Yuan-Agrawal method can seriously compete with other available numerical algorithms.

Chatterjee's variant of the method is amenable to a similar analysis.

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