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HOW TO APPROXIMATE THE FRACTIONAL DERIVATIVE OF ORDER $1 < \alpha \leq 2$

ERCILIA SOUSA
CMUC, Department of Mathematics, University of Coimbra,
3001-454 Coimbra, Portugal
ecs@mat.uc.pt

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The fractional derivative of order α, with $1 < \alpha \leq 2$ appears in several diffusion problems used in physical and engineering applications. Therefore to obtain highly accurate approximations for this derivative is of great importance. Here, we describe and compare different numerical approximations for the fractional derivative of order $1 < \alpha \leq 2$. These approximations arise mainly from the Grünwald–Letnikov definition and the Caputo definition and they are consistent of order one and two. In the end some numerical examples are given, to compare their performance.

Keywords: Diffusion; fractional derivative; finite differences; consistency; accuracy.

1. Introduction

The fractional derivative of order α for $1 < \alpha \leq 2$ in diffusion problems is related to the mechanism of superdiffusion [Zaslavsky, 2002]. There are many analytical techniques to solve fractional differential equations. But in many cases, the reasonable approach is to use numerical methods since the problems have initial conditions, boundary conditions and source terms that become difficult in finding an analytical solution. Different models using fractional derivatives have been proposed and there has been significant interest in developing numerical schemes to find their approximate solution. Some papers where the evidence of fractional diffusion is discussed are, for instance, [Benson *et al.*, 2000; Pachepsky *et al.*, 2000; Zhou & Selim, 2003; Huang *et al.*, 2006].

Many numerical methods involving the fractional derivative that describes diffusion differ essentially in the way the fractional derivative is discretized, see for instance, [Shen & Liu, 2005; Tadjeran *et al.*, 2006; Yuste & Acedo, 2005; Sousa, 2009; Zhang *et al.*, 2007]. Approximations of fractional derivatives have more complex formulas than the approximations of integer derivatives, since the fractional derivative is nonlocal, that is, the calculation at a certain point involves information of the function further out of the region close to that point. Consequently, the finite difference approximations of the fractional derivative involve a number of points that changes according to how far we are from the boundary.

This paper considers the different approaches presented in the literature and compare their truncation errors and order of consistency.

2. Fractional Derivatives

We start to introduce different definitions of the fractional derivative. There are a number of interesting books describing the analytical properties of fractional derivatives, such as, [Kilbas *et al.*, 2006; Oldham & Spanier, 1974; Podlubny, 1999; Samko *et al.*, 1993].

The usual way of representing the fractional derivatives is by the Riemann–Liouville formula.

The Riemann–Liouville fractional derivative of order α, for $x \in [a,b]$, is defined by

$$D^{\alpha}_{\mathrm{RL}} u(x) = \frac{1}{\Gamma(n-\alpha)} \frac{d^n}{dx^n} \int_a^x u(\xi)(x-\xi)^{n-\alpha-1} d\xi, \tag{1}$$

where $\Gamma(\cdot)$ is the Gamma function, $n-1 < \alpha < n$ and $n = [\alpha]+1$, with $[\alpha]$ denoting the integer part of α. Another way to represent the fractional derivatives is by the Grünwald–Letnikov formula, that is, for $\alpha > 0$

$$D^{\alpha}_{\mathrm{GL}} u(x) = \lim_{\Delta x \to 0} \frac{1}{\Delta x^{\alpha}} \sum_{k=0}^{[\frac{x-a}{\Delta x}]} (-1)^k \times \binom{\alpha}{k} u(x - k\Delta x). \tag{2}$$

The Grünwald–Letnikov definition is a generalization of the ordinary discretization formulas for integer order derivatives. If we consider the domain $\mathbb{R}$ the sum in (2) is a series. This series converges absolutely and uniformly for each $\alpha > 0$ and for every bounded function $u(x)$.

The discrete approximations derived from the Grünwald–Letnikov fractional derivative present some limitations. First, they frequently originate unstable numerical methods and henceforth many times a shifted Grünwald–Letnikov formula is used instead, see for instance [Meerschaert & Tadjeran, 2004]. Another disadvantage is that the order of accuracy of such approaches is never higher than one.

A different representation of the fractional derivative was proposed by Caputo,

$$D^{\alpha}_{\mathrm{C}} u(x) = \frac{1}{\Gamma(n-\alpha)} \times \int_a^x \frac{d^n u}{d\xi^n}(\xi)(x-\xi)^{n-\alpha-1} d\xi, \tag{3}$$

where $n-1 < \alpha < n$ and $n = [\alpha]+1$. The Caputo representation has some advantages over the Riemann–Liouville representation. The most well known is related to the fact that very frequently the Laplace transform method is used for solving fractional differential equations. The Laplace transform of the Riemann–Liouville derivative leads to boundary conditions containing the limit values of the Riemann–Liouville fractional derivatives at the lower terminal $x = a$. In spite of the fact that mathematically such problems can be solved, there is no physical interpretation for such type of conditions. On the other hand, the Laplace transform of the Caputo derivative imposes boundary conditions involving integer-order derivatives at the lower point $x = a$ which usually are acceptable physical conditions.

In the next propositions we state that by requiring a reasonable behavior of the function $u(x)$ and its derivatives, we can relate the three definitions. These results can be found respectively in [Podlubny, 1999; Kilbas *et al.*, 2006].

Proposition 1. *Let us assume that the function $u(x)$ is $(n-1)$ times differentiable in $[a,b]$ and that the nth derivative of $u(x)$ is integrable in $[a,b]$. Then, for every $n-1 < \alpha < n$ we have*

$$D^{\alpha}_{\mathrm{GL}} u(x) = D^{\alpha}_{\mathrm{RL}} u(x), \quad a \le x \le b.$$

Proposition 2. *Let us assume that the function $u(x)$ is a function for which the Caputo fractional derivative $D^{\alpha}_{\mathrm{C}} u(x)$ exists together with the Riemman–Liouville fractional derivative $D^{\alpha}_{\mathrm{RL}} u(x)$ in $[a,b]$. Then, for every $n-1 < \alpha < n$ we have, for $a \le x \le b$,*

$$D^{\alpha}_{\mathrm{C}} u(x) = D^{\alpha}_{\mathrm{RL}} u(x) - \sum_{k=0}^{n-1} \frac{d^k u}{dx^k}(a) \frac{(x-a)^{-\alpha+k}}{\Gamma(-\alpha+k+1)}.$$

A modified definition of the Riemann–Liouville derivative was introduced recently by Jumarie [2006]. Although this formulation may not have advantages compared with the Caputo derivative in what concern numerical discretizations, we think it is worth a mention. For $n-1 < \alpha < n$, we get

$$D^{\alpha}_{J} u(x) = \frac{1}{\Gamma(n-\alpha)} \frac{d}{dx} \times \int_a^x \left(\frac{d^{n-1}u}{dx^{n-1}}(\xi) - \frac{d^{n-1}u}{dx^{n-1}}(a) \right) \times (x-\xi)^{n-\alpha-2} d\xi. \tag{4}$$

The main difference is that this definition does not require the existence of the derivative of order n for $u(x)$ as is required by the Caputo derivative.

3. Discretization of the Fractional Derivatives

In this section, we describe different ways of discretizing the fractional derivative.

3.1. *Grünwald–Letnikov approximations*

Let us define the mesh points

$$x_j = a + j\Delta x, \quad j = 0, 1, \ldots, N$$

where Δx denotes the uniform space step.

The Grünwald–Letnikov formulae can lead immediately to the approximation

$$D_{\mathrm{GL}}^{\alpha,\Delta x} u(x_j) = \frac{1}{\Delta x^\alpha} \sum_{k=0}^{j} \omega_k^{(\alpha)} u(x_{j-k}), \tag{5}$$

for

$$\begin{aligned} \omega_k^{(\alpha)} &= (-1)^k \binom{\alpha}{k} \\ &= (-1)^k \frac{\alpha(\alpha-1)\cdots(\alpha-k+1)}{k!} \\ &= \frac{\Gamma(k-\alpha)}{\Gamma(-\alpha)\Gamma(k+1)}. \end{aligned} \tag{6}$$

To implement the fractional difference method, it is necessary to compute the coefficients $\omega_k^{(\alpha)}$, where α is the order of fractional differentiation. For that, we can use the recurrence relationships

$$\omega_0^{(\alpha)} = 1; \quad \omega_k^{(\alpha)} = \left(1 - \frac{\alpha+1}{k}\right)\omega_{k-1}^{(\alpha)}, \quad k = 1, 2, 3, \ldots. \tag{7}$$

This approach is suitable for a fixed value of α. In some problems where α must be found, various values of α need to be considered and this may not be the most appropriated way. Instead of that relation, we can use the fast Fourier transform method.

When discretizing fractional differential equations we observe that in the literature the shifted Grünwald–Letnikov formula is exhaustively used, since, as already mentioned, the numerical approximations based in the unshifted formula very frequently originates unstable numerical methods.

The shifted Grünwald–Letnikov formula is given by

$$D_{\mathrm{GL,S}}^{\alpha,\Delta x} u(x_j) = \frac{1}{\Delta x^\alpha} \sum_{k=0}^{j} \omega_k^{(\alpha)} u(x_{j+1-k}). \tag{8}$$

In the next results we give the leading term of the truncation error for both approaches and observe that although they have the same order of consistency, $\mathcal{O}(\Delta x)$, they are slightly different.

Assuming that $u(x)$ is a function that can be written in the form of a power series

$$u(x) = \sum_{m=0}^{\infty} a_m x^m,$$

we can compare their truncation errors by observing the behavior for each function of the form $u_m(x) = x^m$. The following proof is partially presented in [Podlubny, 1999]. We present it here, since it becomes clearer in the next proof for the shifted Grünwald–Letnikov formula.

Proposition 3. *Let $u_m(x) = x^m, m \geq 0$. Then*

$$\begin{aligned} D_{\mathrm{GL}}^{\alpha,\Delta x} u_0(x) &= D_{\mathrm{GL}}^{\alpha} u_0(x) + \Delta x\ x^{-1-\alpha} \\ &\quad \times \frac{1}{2\Gamma(1-\alpha)}(-\alpha)(-\alpha+1) \\ &\quad + \mathcal{O}(\Delta x^2), \end{aligned} \tag{9}$$

$$\begin{aligned} D_{\mathrm{GL}}^{\alpha,\Delta x} u_m(x) &= D_{\mathrm{GL}}^{\alpha} u_m(x) + \Delta x\ x^{m-1-\alpha} \\ &\quad \times \frac{\Gamma(m+1)}{2\Gamma(m-\alpha)}(-\alpha) + \mathcal{O}(\Delta x^2). \end{aligned} \tag{10}$$

Proof

(a) Let us first consider $m = 0$, that is, $u_0(x) = 1$. We know that

$$D_{\mathrm{GL}}^{\alpha} u_0(x) = \frac{x^{-\alpha}}{\Gamma(1-\alpha)}.$$

For $x = n\Delta x$, we have

$$D_{\mathrm{GL}}^{\alpha,\Delta x} u_0(x) = \frac{1}{\Delta x^\alpha} \sum_{j=0}^{n} (-1)^j \binom{\alpha}{j} u_0(x - j\Delta x).$$

Since [Podlubny, 1999]

$$\sum_{j=0}^{n} (-1)^j \binom{\alpha}{j} = \sum_{j=0}^{n} \binom{j-\alpha-1}{j} = \binom{n-\alpha}{n} \tag{11}$$

we have, for $x = n\Delta x$,

$$\begin{aligned} D_{\mathrm{GL}}^{\alpha,\Delta x} u_0(x) &= \frac{1}{\Delta x^\alpha} \binom{n-\alpha}{n} \\ &= \frac{x^{-\alpha}}{\Gamma(1-\alpha)} n^\alpha \frac{\Gamma(n-\alpha+1)}{\Gamma(n+1)}. \end{aligned}$$

Now using the asymptotic expansion [Abramowitz & Stegun, 1970],

$$\frac{\Gamma(z+a)}{\Gamma(z+b)} = z^{a-b}\left(1+\frac{1}{2}z^{-1}(a-b)(a+b-1)+\mathcal{O}(z^{-2})\right), \tag{12}$$

then

$$D_{\mathrm{GL}}^{\alpha,\Delta x}u_0(x) = \frac{x^{-\alpha}}{\Gamma(1-\alpha)}n^{\alpha}n^{-\alpha} \times\left(1+\frac{1}{2}n^{-1}(-\alpha)(-\alpha+1)+\mathcal{O}(n^{-2})\right).$$

Finally

$$D_{\mathrm{GL}}^{\alpha,\Delta x}u_0(x) = D_{\mathrm{GL}}^{\alpha}u_0(x)+\frac{\Delta x}{2}\frac{x^{-\alpha-1}}{\Gamma(1-\alpha)} \times(-\alpha)(-\alpha+1)+\mathcal{O}(\Delta x^2).$$

Let us now consider $u_m(x) = x^m$ for $m \geq 1$. We know that

$$D_{\mathrm{GL}}^{\alpha}u_m(x) = \frac{\Gamma(1+m)}{\Gamma(1+m-\alpha)}x^{m-\alpha}.$$

For $x = n\Delta x$, we have

$$D_{\mathrm{GL}}^{\alpha,\Delta x}u_m(x) = \frac{1}{\Delta x^{\alpha}}\sum_{j=0}^{n}(-1)^j\binom{\alpha}{j}u_m(x-j\Delta x),$$

that is

$$D_{\mathrm{GL}}^{\alpha,\Delta x}u_m(x) = \frac{1}{\Delta x^{\alpha}}\sum_{j=0}^{n}\binom{j-\alpha-1}{j}(x-j\Delta x)^m = (n\Delta x)^{m-\alpha}n^{\alpha}\sum_{j=0}^{n}\binom{j-\alpha-1}{j} \times\left(1-\frac{j}{n}\right)^m.$$

Expanding the binomial

$$\left(1-\frac{j}{n}\right)^m = \sum_{r=0}^{m}(-1)^r\binom{m}{r}j^r n^{-r}$$

we have

$$D_{\mathrm{GL}}^{\alpha,\Delta x}u_m(x) = x^{m-\alpha}\sum_{r=0}^{m}(-1)^r\binom{m}{r}n^{\alpha-r} \times\sum_{j=0}^{n}\binom{j-\alpha-1}{j}j^r.$$

Let us now rewrite the sum

$$\sum_{j=0}^{n}\binom{j-\alpha-1}{j}j^r.$$

We use the Stirling numbers of the second kind $\sigma_n^{(m)}$ [Abramowitz & Stegun, 1970], that is,

$$x^n = \sum_{i=0}^{n}\sigma_n^{(i)}x^{[i]}, \quad n \geq i, \quad x^{[i]} = \frac{\Gamma(x+1)}{\Gamma(x-i+1)}. \tag{13}$$

In our case, we obtain from (13),

$$j^r = \sum_{i=1}^{r}\sigma_r^{(i)}\frac{\Gamma(j+1)}{\Gamma(j-i+1)}.$$

Therefore,

$$\begin{aligned}\sum_{j=0}^{n}\binom{j-\alpha-1}{j}j^r &= \sum_{i=1}^{r}\sigma_r^{(i)}\sum_{j=i}^{n}\frac{\Gamma(j-\alpha)}{\Gamma(-\alpha)\Gamma(j-i+1)}\\ &= \sum_{i=1}^{r}\sigma_r^{(i)}\sum_{k=0}^{n-i}\frac{\Gamma(k+i-\alpha)}{\Gamma(-\alpha)\Gamma(k+1)}\\ &= \sum_{i=1}^{r}\sigma_r^{(i)}\frac{\Gamma(i-\alpha)}{\Gamma(-\alpha)}\sum_{k=0}^{n-i}\binom{k+i-\alpha-1}{k}.\end{aligned}$$

Now using (11), we can write

$$\begin{aligned}\sum_{j=0}^{n}\binom{j-\alpha-1}{j}j^r &= \sum_{i=1}^{r}\sigma_r^{(i)}\frac{\Gamma(i-\alpha)}{\Gamma(-\alpha)}\binom{n-\alpha}{n-i}\\ &= \sum_{i=1}^{r}\sigma_r^{(i)}\frac{\Gamma(n-\alpha+1)}{(i-\alpha)\Gamma(-\alpha)\Gamma(n-i+1)}\binom{n-\alpha}{n-i}.\end{aligned}$$

Therefore,

$$D_{\mathrm{GL}}^{\alpha,\Delta x} u_m(x) = \frac{x^m}{\Gamma(-\alpha)} \sum_{r=0}^{m} (-1)^r \binom{m}{r} \sum_{i=1}^{r} \sigma_r^{(i)} n^{\alpha-r} \frac{\Gamma(n-\alpha+1)}{(i-\alpha)\Gamma(n-i+1)}.$$

Using (12) we have

$$\begin{aligned} D_{\mathrm{GL}}^{\alpha,\Delta x} u_m(x) &= \frac{x^m}{\Gamma(-\alpha)} \sum_{r=0}^{m} (-1)^r \binom{m}{r} \sum_{i=1}^{r} \sigma_r^{(i)} \frac{n^{i-r}}{i-\alpha} \left(1 + \frac{1}{2} n^{-1}(-\alpha+i)(-\alpha-i+1) + \mathcal{O}(n^{-2})\right) \\ &= \frac{x^{m-\alpha}}{\Gamma(-\alpha)} \sum_{r=0}^{m} (-1)^r \binom{m}{r} \sigma_r^{(r)} \frac{1}{r-\alpha} \left(1 + \frac{1}{2} n^{-1}(-\alpha+r)(-\alpha-r+1) + \mathcal{O}(n^{-2})\right) \\ &\quad + \frac{x^{m-\alpha}}{\Gamma(-\alpha)} \sum_{r=2}^{m} (-1)^r \binom{m}{r} \sum_{i=1}^{r-1} \sigma_r^{(i)} \frac{n^{i-r}}{i-\alpha} \left(1 + \frac{1}{2} n^{-1}(-\alpha+i)(-\alpha-i+1) + \mathcal{O}(n^{-2})\right) \\ &= \frac{x^{m-\alpha}}{\Gamma(-\alpha)} \sum_{r=0}^{m} (-1)^r \binom{m}{r} \frac{\sigma_r^{(r)}}{r-\alpha} + \frac{1}{2} \frac{x^{m-\alpha}}{\Gamma(-\alpha)} \sum_{r=0}^{m} (-1)^r \binom{m}{r} \frac{\sigma_r^{(r)}}{r-\alpha} n^{-1}(-\alpha+r)(-\alpha-r+1) \\ &\quad + \frac{x^{m-\alpha}}{\Gamma(-\alpha)} \sum_{r=2}^{m} (-1)^r \binom{m}{r} \sigma_r^{(r-1)} \frac{n^{-1}}{r-1-\alpha} + \mathcal{O}(n^{-2}). \end{aligned}$$

Since $\sigma_r^{(r)} = 1$ and as we have found in [Podlubny, 1999],

$$\sum_{r=0}^{m} (-1)^r \binom{m}{r} \frac{1}{r-\alpha} = \frac{\Gamma(1+m)\Gamma(-\alpha)}{\Gamma(1+m-\alpha)} \quad (14)$$

we have,

$$\begin{aligned} D_{\mathrm{GL}}^{\alpha,\Delta x} u_m(x) &= D_{\mathrm{GL}}^{\alpha} u_m(x) + \Delta x \frac{1}{2} \frac{x^{m-\alpha-1}}{\Gamma(-\alpha)} \\ &\quad \times \sum_{r=0}^{m} (-1)^r \binom{m}{r} (-\alpha-r+1) \\ &\quad + \Delta x \frac{x^{m-\alpha-1}}{\Gamma(-\alpha)} \sum_{r=2}^{m} (-1)^r \binom{m}{r} \sigma_r^{(r-1)} \\ &\quad \times \frac{1}{r-1-\alpha} + \mathcal{O}(\Delta x^2), \end{aligned}$$

where $\sigma_r^{(r-1)} = \binom{r}{2}$. It is also easy to prove that

$$\sum_{r=0}^{m} (-1)^r \binom{m}{r} (-\alpha-r+1) = 0;$$

$$\sum_{r=0}^{m} (-1)^r \binom{m}{r} \frac{r(r-1)}{r-1-\alpha} = \frac{\Gamma(m+1)\Gamma(1-\alpha)}{\Gamma(m-\alpha)}. \quad (15)$$

Therefore we have,

$$\begin{aligned} D_{\mathrm{GL}}^{\alpha,\Delta x} u_m(x) &= D_{\mathrm{GL}}^{\alpha} u_m(x) + \Delta x \frac{1}{2} \frac{x^{m-\alpha-1}}{\Gamma(-\alpha)} \\ &\quad \times \frac{\Gamma(m+1)\Gamma(1-\alpha)}{\Gamma(m-\alpha)} + \mathcal{O}(\Delta x^2), \end{aligned}$$

and then we get (10). ■

We now turn to the shifted formula.

Proposition 4. *Let* $u_m(x) = x^m, m \geq 0$. *Then*

$$\begin{aligned} D_{\mathrm{GL,S}}^{\alpha,\Delta x} u_0(x) &= D_{\mathrm{GL}}^{\alpha} u_0(x) + \Delta x\ x^{-1-\alpha} \\ &\quad \times \frac{1}{2\Gamma(1-\alpha)} (-\alpha)(-\alpha+3) \\ &\quad + \mathcal{O}(\Delta x^2), \end{aligned} \quad (16)$$

$$\begin{aligned} D_{\mathrm{GL,S}}^{\alpha,\Delta x} u_m(x) &= D_{\mathrm{GL}}^{\alpha} u_m(x) + \Delta x\ x^{m-1-\alpha} \\ &\quad \times \frac{\Gamma(m+1)}{2\Gamma(m-\alpha)} (2-\alpha) + \mathcal{O}(\Delta x^2). \end{aligned} \quad (17)$$

Proof. Let us first consider $m = 0$, that is, $u_0(x) = 1$. For $x = n\Delta x$, we have

$$D_{\mathrm{GL,S}}^{\alpha,\Delta x}u_0(x)=\frac{1}{\Delta x^\alpha}\sum_{j=0}^{n+1}(-1)^j\binom{\alpha}{j}\times u_0(x-j\Delta x+\Delta x).$$

Then,

$$D_{\mathrm{GL,S}}^{\alpha,\Delta x}u_0(x)=\frac{1}{\Delta x^\alpha}\binom{n+1-\alpha}{n+1}=\frac{x^{-\alpha}}{\Gamma(1-\alpha)}n^\alpha\frac{\Gamma(n-\alpha+2)}{\Gamma(n+2)}.$$

From (12),

$$D_{\mathrm{GL,S}}^{\alpha,\Delta x}u_0(x)=\frac{x^{-\alpha}}{\Gamma(1-\alpha)}n^\alpha n^{-\alpha}\times\left(1+\frac{1}{2}n^{-1}(-\alpha)(-\alpha+3)+\mathcal{O}(n^{-2})\right).$$

Finally

$$D_{\mathrm{GL,S}}^{\alpha,\Delta x}u_0(x)=D_{\mathrm{GL}}^{\alpha}u_0(x)+\frac{\Delta x}{2}x^{-\alpha-1}\times\frac{1}{\Gamma(1-\alpha)}(-\alpha)(-\alpha+3)+\mathcal{O}(\Delta x^2).$$

For $u_m(x)=x^m$ we have

$$D_{\mathrm{GL,S}}^{\alpha,\Delta x}u_m(x)=\frac{1}{\Delta x^\alpha}\sum_{j=0}^{n+1}(-1)^j\binom{\alpha}{j}\times u_m(x-j\Delta x+\Delta x),$$

that is,

$$\begin{aligned}D_{\mathrm{GL,S}}^{\alpha,\Delta x}u_m(x)&=\frac{1}{\Delta x^\alpha}\sum_{j=0}^{n+1}\binom{j-\alpha-1}{j}(x-j\Delta x+\Delta x)^m\\&=(n+1)^m\Delta x^{m-\alpha}\sum\binom{j-\alpha-1}{j}\times\left(1-\frac{j}{n+1}\right)^m.\end{aligned}$$

Expanding the binomial we obtain

$$D_{\mathrm{GL,S}}^{\alpha,\Delta x}u_m(x)=(n+1)^m\Delta x^{m-\alpha}\sum_{r=0}^{m}(-1)^r\binom{m}{r}\times(n+1)^{-r}\sum_{j=0}^{n+1}\binom{j-\alpha-1}{j}j^r.$$

Let us now rewrite the sum

$$\sum_{j=0}^{n+1}\binom{j-\alpha-1}{j}j^r.$$

We use the Stirling numbers of the second kind $\sigma_n^{(m)}$, as previously in (13), to get

$$\sum_{j=0}^{n}\binom{j-\alpha-1}{j}j^r=\sum_{i=1}^{r}\sigma_r^{(i)}\frac{\Gamma(i-\alpha)}{\Gamma(-\alpha)}\binom{n+1-\alpha}{n+1-i}.$$

Therefore,

$$D_{\mathrm{GL}}^{\alpha,\Delta x}u_m(x)=(n+1)^m\frac{\Delta x^{m-\alpha}}{\Gamma(-\alpha)}\sum_{r=0}^{m}(-1)^r\binom{m}{r}(n+1)^{-r}\sum_{i=1}^{r}\sigma_r^{(i)}\frac{\Gamma(n-\alpha+2)}{(i-\alpha)\Gamma(n-i+2)}.$$

Using (12) we have

$$D_{\mathrm{GL,S}}^{\alpha,\Delta x}u_m(x)=(n+1)^m\frac{\Delta x^{m-\alpha}}{\Gamma(-\alpha)}\sum_{r=0}^{m}(-1)^r\binom{m}{r}(n+1)^{-r}\sum_{i=1}^{r}\frac{\sigma_r^{(i)}}{i-\alpha}(n+1)^{-\alpha+i}\times\left(1+\frac{1}{2}(n+1)^{-1}(-\alpha+i)(-\alpha-i+2)+\mathcal{O}((n+1)^{-2})\right).$$

Consider

$$D_{\mathrm{GL}}^{\alpha,\Delta x}u_m(x)=A_1+A_2,$$

for

$$A_1=(n+1)^{m-\alpha}\frac{\Delta x^{m-\alpha}}{\Gamma(-\alpha)}\sum_{r=0}^{m}(-1)^r\binom{m}{r}\frac{\sigma_r^{(r)}}{r-\alpha}\left(1+\frac{1}{2}(n+1)^{-1}(-\alpha+r)(-\alpha-r+2)+\mathcal{O}((n+1)^{-2})\right),$$

$$A_2 = (n+1)^m \frac{\Delta x^{m-\alpha}}{\Gamma(-\alpha)} \sum_{r=2}^{m} (-1)^r \binom{m}{r} (n+1)^{-r} \sum_{i=1}^{r-1} \frac{\sigma_r^{(i)}}{i-\alpha} (n+1)^{-\alpha+i}$$
$$\times \left(1 + \frac{1}{2}(n+1)^{-1}(-\alpha+i)(-\alpha-i+2) + \mathcal{O}((n+1)^{-2})\right).$$

For A_1 we have

$$A_1 = \left(\frac{n+1}{n}\right)^{m-\alpha} n^{m-\alpha} \frac{\Delta x^{m-\alpha}}{\Gamma(-\alpha)} \sum_{r=0}^{m} (-1)^r \binom{m}{r} \frac{\sigma_r^{(r)}}{r-\alpha} + \left(\frac{n+1}{n}\right)^{m-\alpha-1} n^{m-\alpha-1} \frac{\Delta x^{m-\alpha}}{\Gamma(-\alpha)}$$
$$\times \sum_{r=0}^{m} (-1)^r \binom{m}{r} \frac{\sigma_r^{(r)}}{r-\alpha} \frac{1}{2}(-\alpha+r)(-\alpha-r+2) + \mathcal{O}((n+1)^{-2}).$$

It is easy to check that $\mathcal{O}((n+1)^{-2}) = \mathcal{O}(\Delta x^2)$ for a fixed x. Then

$$A_1 = \left(1 + \frac{m-\alpha}{n} + \mathcal{O}(n^{-2})\right)\left(\frac{x^{m-\alpha}}{\Gamma(-\alpha)} \sum_{r=0}^{m} (-1)^r \binom{m}{r} \frac{\sigma_r^{(r)}}{r-\alpha}\right) + \left(1 + \frac{m-\alpha-1}{n} + \mathcal{O}(n^{-2})\right)$$
$$\times \Delta x \frac{x^{m-\alpha-1}}{\Gamma(-\alpha)} \sum_{r=0}^{m} (-1)^r \binom{m}{r} \frac{\sigma_r^{(r)}}{r-\alpha} \frac{1}{2}(-\alpha+r)(-\alpha-r+2) + \mathcal{O}(\Delta x^2)$$
$$= \frac{x^{m-\alpha}}{\Gamma(-\alpha)} \sum_{r=0}^{m} (-1)^r \binom{m}{r} \frac{\sigma_r^{(r)}}{r-\alpha} + \Delta x \frac{x^{m-\alpha-1}}{\Gamma(-\alpha)} (m-\alpha) \sum_{r=0}^{m} (-1)^r \binom{m}{r} \frac{\sigma_r^{(r)}}{r-\alpha}$$
$$+ \Delta x \frac{x^{m-\alpha-1}}{\Gamma(-\alpha)} \sum_{r=0}^{m} (-1)^r \binom{m}{r} \frac{1}{2}(-\alpha-r+2) + \mathcal{O}(\Delta x^2).$$

Now we turn to A_2. We have, using similar tools,

$$A_2 = \left(\frac{n+1}{n}\right)^{m-\alpha} n^{m-\alpha} \frac{\Delta x^{m-\alpha}}{\Gamma(-\alpha)} \sum_{r=2}^{m} (-1)^r \binom{m}{r} \sigma_r^{(r-1)} \frac{(n+1)^{-1}}{r-1-\alpha}$$
$$\times \left(1 + \frac{1}{2}(n+1)^{-1}(-\alpha+r-1)(-\alpha-r+3) + \mathcal{O}(\Delta x^2)\right)$$
$$= \Delta x \frac{\Delta x^{m-\alpha-1}}{\Gamma(-\alpha)} \sum_{r=2}^{m} (-1)^r \binom{m}{r} \frac{\sigma_r^{(r-1)}}{r-1-\alpha} + \mathcal{O}(\Delta x^2),$$

where $\sigma_r^{(r-1)} = \binom{r}{2}$. Then,

$$D_{\mathrm{GL,S}}^{\alpha,\Delta x} u_m(x) = D_{\mathrm{GL}}^{\alpha} u_m(x) + \Delta x \frac{x^{m-\alpha-1}}{\Gamma(-\alpha)} (m-\alpha) \sum_{r=0}^{m} (-1)^r \binom{m}{r} \frac{1}{r-\alpha} + \Delta x \frac{x^{m-\alpha-1}}{\Gamma(-\alpha)}$$
$$\times \sum_{r=0}^{m} (-1)^r \binom{m}{r} \frac{1}{2}(-\alpha-r+2) + \Delta x \frac{\Delta x^{m-\alpha-1}}{\Gamma(-\alpha)} \sum_{r=2}^{m} (-1)^r \binom{m}{r} \frac{\sigma_r^{(r-1)}}{r-1-\alpha} + \mathcal{O}(\Delta x^2).$$

Finally, using (14) and (15) we have

$$D_{\mathrm{GL,S}}^{\alpha,\Delta x}u_m(x) = D_{\mathrm{GL}}^{\alpha}u_m(x) + \Delta x\frac{x^{m-\alpha-1}}{\Gamma(-\alpha)}(m-\alpha)\frac{\Gamma(m+1)\Gamma(-\alpha)}{\Gamma(m+1-\alpha)} + \Delta x\frac{\Delta x^{m-\alpha-1}}{\Gamma(-\alpha)}\frac{1}{2}\frac{\Gamma(m+1)\Gamma(1-\alpha)}{\Gamma(m-\alpha)} + \mathcal{O}(\Delta x^2),$$

and we obtain (17). ■

3.2. *Lubich approximations*

The coefficients $\omega_k^{(\alpha)}$ on Eqs. (5) and (8) can be considered as the coefficients of the power series for the function $(1-z)^\alpha$

$$(1-z)^\alpha = \sum_{k=0}^{\infty}\omega_k^{(\alpha)}z^k, \tag{18}$$

as noted in [Lubich, 1986]. We can say, for instance, that in (5) the weights $\omega_k^{(\alpha)}$ assigned to the values $u(x-k\Delta x)$, are the first order $N+1$ coefficients of the Taylor series expansion of the function

$$f_1^\alpha(z) = (1-z)^\alpha. \tag{19}$$

Lubich [1986] obtained approximations up to the sixth order in the form

$$D_{\mathrm{L}}^{\alpha,\Delta x}u(x_j) = \frac{1}{\Delta x^\alpha}\sum_{k=0}^{j}\omega_k^{(\alpha)}u(x_{j-k}) + \frac{1}{\Delta x^\alpha}\sum_{k=0}^{s}\omega_{jk}^{(\alpha)}u(x_k). \tag{20}$$

The coefficients $\omega_k^{(\alpha)}$ are respectively the coefficients of the Taylor series expansions of the corresponding generating functions, $f_p(z)$, p being the order of consistency. For $p=2$, the function is given by

$$f_2^\alpha(z) = \left(\frac{3}{2} - 2z + \frac{1}{2}z^2\right)^\alpha. \tag{21}$$

Technically all the coefficients $\omega_k^{(\alpha)}$ can be computed using any implementation of the fast Fourier transform.

For the coefficients $\omega_{jk}^{(\alpha)}$ we can consider $s=0$. For $s\neq 0$, the coefficients $\omega_{jk}^{(\alpha)}$ can be constructed such that

$$D_{\mathrm{RL}}^{\alpha}(x_j)^q = D_{\mathrm{L}}^{\alpha,\Delta x}(x_j)^q, \quad \text{for all integer } 0\le q\le p-1,$$

which results in the following system of equations

$$\sum_{k=1}^{s}\omega_{jk}^{(\alpha)}k^q = \frac{\Gamma(q+1)}{\Gamma(-\alpha+q+1)}j^{q-\alpha} - \sum_{k=1}^{j}\omega_{j-k}^{(\alpha)}k^q, \quad q=0,\ldots,s-1.$$

It is easy to see that in this case it makes sense to choose $s=p$.

The implementation of the fast Fourier transform consist of the following. If $f(z)$ is an analytic function in the closed unit disk, then its Taylor series converges there, and the Taylor coefficients can be computed by Cauchy integrals:

$$f(z) = \sum_{k=0}^{\infty}a_k z^k, \quad a_k = \frac{1}{2\pi i}\int_{|z|=1} z^{-k-1}f(z)dz, \tag{22}$$

where the contour of integration is the unit circle traversed once counterclockwise.

Setting $z=e^{i\phi}$, with $dz = izd\phi$ shows that an equivalent expression for a_k is

$$a_k = \frac{1}{2\pi}\int_0^{2\pi} e^{-ik\phi}f(e^{i\phi})d\phi. \tag{23}$$

These coefficients can be evaluated by the fast Fourier transform.

In our particular case, the analytic function $f_p^\alpha(z)$ is

$$f_p^\alpha(e^{i\phi}) = \sum_{k=0}^{\infty}\omega_k^{(\alpha)}e^{i\phi k}, \quad p=1,2, \tag{24}$$

with the coefficients given by

$$\omega_k^{(\alpha)} = \frac{1}{2\pi}\int_0^{2\pi} e^{-ik\phi}f_p^\alpha(e^{i\phi})d\phi. \tag{25}$$

Note that for $\alpha = 2$ the coefficients $\omega_k^{(\alpha)}$ can be easily obtained. For instance, for $p = 1$

$$\omega_0^{(2)} = 1, \quad \omega_1^{(2)} = -2, \quad \omega_2^{(2)} = 1,$$

$$\omega_k^{(2)} = 0, \quad k \geq 3,$$

and for $p = 2$

$$\omega_0^{(2)} = \frac{9}{4}, \quad \omega_1^{(2)} = -6, \quad \omega_2^{(2)} = \frac{11}{2}, \quad \omega_3^{(2)} = -2,$$

$$\omega_4^{(2)} = \frac{1}{4}, \quad \omega_k^{(2)} = 0, \quad k \geq 5.$$

According to Lubich [1986], we have the following result.

Proposition 5. *For any function* $u(x)$ *sufficiently differentiable, the approximation* $D_{\mathrm{L}}^{\alpha,\Delta x}u(x_j)$, *satisfies*

$$D_{\mathrm{L}}^{\alpha,\Delta x}u(x_j) - D_{\mathrm{RL}}^{\alpha}u(x_j) = \mathcal{O}(\Delta x^p).$$

uniformly for $x_j \in [a, b]$, $0 < a < b < \infty$.

3.3. *Caputo approximations*

In this section we derive numerical approximations based on the Caputo derivative definition,

$$D_{\mathrm{C}}^{\alpha}u(x) = \frac{1}{\Gamma(2-\alpha)}\int_a^x \frac{d^2u}{d\xi^2}(\xi)(x-\xi)^{1-\alpha}d\xi. \quad (26)$$

For each x_j, we have that

$$D_{\mathrm{C}}^{\alpha}u(x_j) = \frac{1}{\Gamma(2-\alpha)}\sum_{k=0}^{j-1}\int_{x_k}^{x_{k+1}} \frac{d^2u}{d\xi^2}(\xi)(x_j-\xi)^{1-\alpha}d\xi. \quad (27)$$

An usual way of approximating the Caputo derivative $D_{\mathrm{C}}^{\alpha}u(x_j)$ is by

$$\begin{aligned} D_{\mathrm{C},1}^{\alpha,\Delta x}u(x_j) &= \frac{1}{\Gamma(2-\alpha)}\sum_{k=0}^{j-1}\frac{u(x_{k+2}) - 2u(x_{k+1}) + u(x_k)}{\Delta x^2}\int_{x_k}^{x_{k+1}}(x_j-\xi)^{1-\alpha}d\xi \\ &= \frac{1}{\Gamma(2-\alpha)}\sum_{k=0}^{j-1}\frac{u(x_{k+2}) - 2u(x_{k+1}) + u(x_k)}{\Delta x^2}\frac{\Delta x^{2-\alpha}}{2-\alpha}d_{j,k} \\ &= \frac{\Delta x^{-\alpha}}{\Gamma(3-\alpha)}\sum_{k=0}^{j-1}d_{j,k}(u(x_{k+2}) - 2u(x_{k+1}) + u(x_k)), \end{aligned}$$

for

$$d_{j,k} = (j-k)^{2-\alpha} - (j-k-1)^{2-\alpha}.$$

This is a first order approximation as stated in the next result and proved in [Shen & Liu, 2005].

Proposition 6. *Let* $u(x)$ *be a function in* $C^3[a, b]$ *and* $1 < \alpha < 2$. *Then*

$$D_{\mathrm{C},1}^{\alpha,\Delta x}u(x_j) = D_{\mathrm{C},1}^{\alpha}u(x_j) + E_{\mathrm{C},1}(x_j)$$

with

$$|E_{\mathrm{C},1}(x_j)| \leq \frac{2(x_j-a)^{2-\alpha}}{\Gamma(3-\alpha)}\mathcal{O}(\Delta x).$$

Let us now derive a second order approximation. For x_j, $j = 1, \ldots, N-1$ we need to calculate

$$\frac{1}{\Gamma(2-\alpha)}\int_a^{x_j}\frac{d^2u}{d\xi^2}(\xi)(x_j-\xi)^{1-\alpha}d\xi. \quad (28)$$

We compute these integrals by approximating the second order derivative by a linear spline $s_j(\xi)$, whose nodes and knots are chosen at x_k, $k = 0, 1, 2, \ldots, j$. A similar approach is done in [Diethelm *et al.*, 2004a, 2004b; Li & Tao, 2009; Li *et al.*, 2011]. The spline $s_j(\xi)$ is of the form

$$s_j(\xi) = \sum_{k=0}^{j}\frac{d^2u}{d\xi^2}(x_k)s_{j,k}(\xi), \quad (29)$$

with $s_{j,k}(\xi)$, in each interval $[x_{k-1}, x_{k+1}]$, for $1 \leq k \leq j-1$, given by

$$s_{j,k}(\xi) = \begin{cases} \dfrac{\xi - x_{k-1}}{x_k - x_{k-1}}, & x_{k-1} \leq \xi \leq x_k \\ \dfrac{x_{k+1} - \xi}{x_{k+1} - x_k}, & x_k \leq \xi \leq x_{k+1} \\ 0 & \text{otherwise.} \end{cases}$$

For $k = 0$ and $k = j$, $s_{j,k}(\xi)$ is of the form

$$s_{j,0}(\xi) = \begin{cases} \dfrac{x_1 - \xi}{x_1 - x_0}, & x_0 \leq \xi \leq x_1 \\ 0 & \text{otherwise} \end{cases}$$

$$s_{j,j}(\xi) = \begin{cases} \dfrac{\xi - x_{j-1}}{x_j - x_{j-1}}, & x_{j-1} \leq \xi \leq x_j \\ 0 & \text{otherwise.} \end{cases}$$

Therefore, an approximation for (28) is of the form

$$\frac{1}{\Gamma(2-\alpha)} \int_a^{x_j} s_j(\xi)(x_j - \xi)^{1-\alpha} d\xi$$
$$= \frac{1}{\Gamma(2-\alpha)} \sum_{k=0}^{j} \frac{d^2u}{d\xi^2}(x_k) \times \int_a^{x_j} (x_j - \xi)^{1-\alpha} s_{j,k}(\xi) d\xi,$$

and after some calculations we obtain

$$\frac{1}{\Gamma(2-\alpha)} \int_a^{x_j} s_j(\xi)(x_j - \xi)^{1-\alpha} d\xi = \frac{\Delta x^{2-\alpha}}{\Gamma(4-\alpha)} \sum_{k=0}^{j} \frac{d^2u}{d\xi^2}(x_k) a_{j,k}, \tag{30}$$

where

$$a_{j,k} = (j-1)^{3-\alpha} - j^{2-\alpha}(j - 3 + \alpha), \quad k = 0 \tag{31}$$

$$a_{j,k} = (j-k+1)^{3-\alpha} - 2(j-k)^{3-\alpha} + (j-k-1)^{3-\alpha}, \quad 1 \leq k \leq j-1 \tag{32}$$

$$a_{j,k} = 1, \quad k = j. \tag{33}$$

For the mesh points x_k, $k = 1, \ldots, N-1$ the second order derivative of (30) can be approximated by $\delta^2 u_j/\Delta x^2$ where δ^2 is the central second order differential operator

$$\delta^2 u_j = u(x_{j+1}) - 2u(x_j) + u(x_{j-1}).$$

Additionally, we also need to know the value of the second order derivative at the boundary point x_0. If we have a physical boundary condition of the type

$$\frac{d^2u}{dx^2}(x_0) = b_0 \tag{34}$$

we can consider the given value. If this value is not available at $x = x_0$ the second order derivative can be approximated by $\delta_0 U_0/\Delta x^2$ where δ_0 is the operator

$$\delta_0 u_j = 2u(x_j) - 5u(x_{j+1}) + 4u(x_{j+2}) - u(x_{j+3}). \tag{35}$$

Finally, an approximation for $D_{\mathrm{C}}^{\alpha}(x_j)$ can be written as

$$D_{\mathrm{C}}^{\alpha,\Delta x} u(x_j) = \frac{\Delta x^{-\alpha}}{\Gamma(4-\alpha)} \left\{ a_{j,0}\delta_0 u_0 + \sum_{k=1}^{j} a_{j,k}\delta^2 u_k \right\}.$$

We have the following result, proved in [Sousa, 2011].

Proposition 7. *Let $u(x)$ be a function in $C^4[a,b]$ and $1 < \alpha < 2$. Then*

$$D_{\mathrm{C}}^{\alpha,\Delta x} u(x_j) = D_{\mathrm{C}}^{\alpha} u(x_j) + E_{\mathrm{C}}(x_j)$$

with

$$|E_{\mathrm{C}}(x_j)| \leq \frac{2(x_j - a)^{2-\alpha}}{\Gamma(3-\alpha)} \mathcal{O}(\Delta x^2).$$

Note that

$$D_{\mathrm{C}}^{\alpha} u(x) = D_{\mathrm{RL}}^{\alpha} u(x) - \sum_{k=0}^{1} \frac{d^k u}{dx^k}(a) \frac{(x-a)^{-\alpha+k}}{\Gamma(-\alpha+k+1)},$$

that is

$$D_{\mathrm{RL}}^{\alpha} u(x) = D_{\mathrm{C}}^{\alpha} u(x) + u(a) \frac{(x-a)^{-\alpha}}{\Gamma(-\alpha+1)} + u'(a) \frac{(x-a)^{-\alpha+1}}{\Gamma(-\alpha+2)}.$$

If we want a first order approximation for the derivative $D_{\mathrm{RL}}^{\alpha} u(x)$, we can use a first order approximation to determine $u'(a)$ by using the forward operator

$$\Delta_+ u(x_j) = u(x_{j+1}) - u(x_j)$$

and

$$u'(x_j) = \frac{\Delta_+ u(x_j)}{\Delta x} + \mathcal{O}(\Delta x).$$

On the other hand if we want a second order approximation for the Riemman–Liouville derivative we can use the second order approximation for the first derivative, such as,

$$u'(x_j) = \frac{-u(x_{j+2}) + 4u(x_{j+1}) - 3u(x_j)}{2\Delta x} + \mathcal{O}(\Delta x^2).$$

4. Numerical Tests

In this section, we present some numerical results. The magnitude of the truncation error is compared for the approximations discussed previously and their order of consistency is confirmed.

4.1. *Boundary conditions are zero*

Consider the function $u(x) = x^4$. We have that, for $1 < \alpha \leq 2$,

$$D_{\mathrm{C}}^{\alpha} u(x) = D_{\mathrm{RL}}^{\alpha} u(x) = D_{\mathrm{GL}}^{\alpha} u(x) = \frac{24}{\Gamma(5-\alpha)} x^{4-\alpha}.$$

Consider the vectors $U_{\mathrm{app}} = (U(x_0), \ldots, U(x_N))$, where U is the approximate solution and $u_{\mathrm{ex}} = (u(x_0), \ldots, u(x_N))$, where u is the exact solution. The error is defined by

$$\|u_{\mathrm{ex}}(\Delta x) - U_{\mathrm{app}}(\Delta x)\|_{\infty}, \tag{36}$$

where $\|\cdot\|_{\infty}$ is the l_{∞} norm.

In Table 1 we compare the first order approximations and in Table 2 we compare the second order approximations for $\alpha = 1.8$. We observe in Table 1, that the approximation based on the shifted Grünwald–Letnikov formula gives the smaller error. This is in agreement with the theoretical results (10) and (17). In Table 2, the approximation based on the Caputo derivative performs better.

Table 1. l_{∞} error (36) for $\alpha = 1.8$, $0 \leq x \leq 1$.

Δx	$D_{\mathrm{GL}}^{\alpha,\Delta x}$	$D_{\mathrm{GL,S}}^{\alpha,\Delta x}$	$D_{\mathrm{C,1}}^{\alpha,\Delta x}$
$\frac{1}{50}$	0.3778×10^{0}	0.4335×10^{-1}	0.1327×10^{0}
$\frac{1}{500}$	0.3903×10^{-1}	0.4385×10^{-2}	0.1648×10^{-1}
$\frac{1}{5000}$	0.3919×10^{-2}	0.4356×10^{-3}	0.1845×10^{-2}

Table 2. l_{∞} error (36) for $\alpha = 1.8$, $0 \leq x \leq 1$.

Δx	$D_{\mathrm{L}}^{\alpha,\Delta x}$	$D_{\mathrm{C}}^{\alpha,\Delta x}$
$\frac{1}{50}$	0.6229×10^{-2}	0.1496×10^{-2}
$\frac{1}{500}$	0.5421×10^{-4}	0.1602×10^{-4}
$\frac{1}{5000}$	0.2511×10^{-2}	0.1678×10^{-6}

Table 3. l_{∞} error (36) for $\alpha = 1.2$, $0 \leq x \leq 1$.

Δx	$D_{\mathrm{GL}}^{\alpha,\Delta x}$	$D_{\mathrm{GL,S}}^{\alpha,\Delta x}$	$D_{\mathrm{C,1}}^{\alpha,\Delta x}$
$\frac{1}{50}$	0.1633×10^{0}	0.1118×10^{0}	0.1379×10^{0}
$\frac{1}{500}$	0.1697×10^{-1}	0.1142×10^{-1}	0.1425×10^{-1}
$\frac{1}{5000}$	0.1717×10^{-2}	0.1145×10^{-2}	0.1431×10^{-2}

Additionally, the approximation $D_{\mathrm{L}}^{\alpha,\Delta x} u(x)$ starts to perform well for values of $\Delta x = 1/50$ and $\Delta x = 1/500$ but for quite small Δx, such as, $\Delta x = 1/5000$ we have accuracy problems. Numerical problems related to this approximation are also reported, for instance, in [Diethelm *et al.*, 2004]. Note that for this approximation we have considered $s = 0$ in (20), since there was no significant differences in the precision if we consider $s = 1$.

In Tables 3 and 4, we do similar tests to the ones that were done in Tables 1 and 2, but now for $\alpha = 1.2$. The conclusions are the same.

4.2. *Nonzero boundary conditions*

Let us now consider for $0 \leq x < 1$, the function

$$u(x) = \frac{x}{(1-x)^{5/2}},$$

and $\alpha = 3/2$. We have that

$$D_{\mathrm{RL}}^{\alpha} u(x) = \frac{3x^2 + 18x + 3}{\Gamma\left(\frac{5}{2}\right)\sqrt{x}(1-x)^4}.$$

Note that

$$u'(x) = \frac{2+3x}{2(1-x)^{7/2}} \quad u''(x) = \frac{20+15x}{4(1-x)^{9/2}}$$

and therefore

$$u(0) = 0 \quad u'(0) = 1 \quad u''(0) = 5.$$

Table 4. l_{∞} error (36) for $\alpha = 1.2$, $0 \leq x \leq 1$.

Δx	$D_{\mathrm{L}}^{\alpha,\Delta x}$	$D_{\mathrm{C}}^{\alpha,\Delta x}$
$\frac{1}{50}$	0.4006×10^{-2}	0.1606×10^{-2}
$\frac{1}{500}$	0.8689×10^{-4}	0.1707×10^{-4}
$\frac{1}{5000}$	0.4160×10^{-2}	0.1716×10^{-6}

Table 5. First order error for $\alpha = 1.5$ at $x = 1/4$.

Δx	$D^{\alpha,\Delta x}_{\mathrm{GL,S}} u(1/4)$	Error
$\frac{1}{60}$	9.372416532513057	0.2339×10^{0}
$\frac{1}{600}$	9.160930732981797	0.2245×10^{-1}
$\frac{1}{6000}$	9.140714295237558	0.2236×10^{-2}

The solution, $D^{\alpha}_{\mathrm{RL}} u(1/4)$, at $x = 1/4$, and considering sixteen digits, is given by $D^{\alpha}_{\mathrm{RL}} u(1/4) = 9.138478192773535$.

In Tables 5 and 6 we compare the two approximations based on the Grünwald–Letnikov definition and its confirmed that the shifted formula gives smaller errors and we note again this is in agreement with the theoretical results (10) and (17).

Since the first order derivative at the left boundary is not zero, the Caputo derivative and the Riemann–Liouville derivative are different. In the next tables we present the Riemman–Liouville derivative values based on the Caputo approximations.

The approximations of the first order and second order derivatives at the boundary point must be considered as described in the previous section, that is, to obtain a first order approximation for the Riemman–Liouville derivative, and assuming $u(0) = 0$ we need to consider the approximation,

$$D^{\alpha,\Delta x}_{\mathrm{RL},1} u(x_j) = D^{\alpha,\Delta x}_{\mathrm{C},1} u(x_j) + \frac{u(x_1) - u(x_0)}{\Delta x} \times \frac{x_j^{-\alpha+1}}{\Gamma(-\alpha+2)},$$

and to obtain a second order approximation,

$$D^{\alpha,\Delta x}_{\mathrm{RL}} u(x_j) = D^{\alpha,\Delta x}_{\mathrm{C}} u(x_j) + \frac{-u(x_2) + 4u(x_1) - 3u(x_0)}{2\Delta x} \times \frac{x_j^{-\alpha+1}}{\Gamma(-\alpha+2)}. \tag{37}$$

Table 6. First order error for $\alpha = 1.5$ at $x = 1/4$.

Δx	$D^{\alpha,\Delta x}_{\mathrm{GL}} u(1/4)$	Error
$\frac{1}{60}$	8.504256221012128	0.6342×10^{0}
$\frac{1}{600}$	9.071845197716357	0.6663×10^{-1}
$\frac{1}{6000}$	9.138478192773535	0.6701×10^{-2}

Table 7. First order error for $\alpha = 1.5$ at $x = 1/4$.

Δx	$D^{\alpha,\Delta x}_{\mathrm{RL},1} u(1/4)$	Error
$\frac{1}{60}$	9.557038359800762	0.4186×10^{0}
$\frac{1}{600}$	9.183034203064997	0.4456×10^{-1}
$\frac{1}{6000}$	9.143066643085710	0.4588×10^{-2}

Table 8. Second order error for $\alpha = 1.5$ at $x = 1/4$.

Δx	$D^{\alpha,\Delta x}_{\mathrm{RL}} u(1/4)$	Error
$\frac{1}{60}$	9.151374640108251	0.1290×10^{-1}
$\frac{1}{600}$	9.138618733987558	0.1405×10^{-3}
$\frac{1}{6000}$	9.138479620502642	0.1428×10^{-5}

In Tables 7 and 8 we show the performance of the derivatives $D^{\alpha,\Delta x}_{\mathrm{RL},1} u(x)$ and $D^{\alpha,\Delta x}_{\mathrm{RL}} u(x)$ and see that the approximation $D^{\alpha,\Delta x}_{\mathrm{RL}} u(x)$ is quite accurate.

Finally we present the results for the derivative based on the second order Lubich approximation and it is again confirmed that for quite small space steps we have precision problems.

We conclude the second order approximation based on the Caputo definition is a very good option.

Table 9. Second order error for $\alpha = 1.5$ at $x = 1/4$.

Δx	$D^{\alpha,\Delta x}_{\mathrm{L}} u(1/4)$	Error
$\frac{1}{60}$	9.087659189694477	0.5082×10^{-1}
$\frac{1}{600}$	9.137964592304343	0.5136×10^{-3}
$\frac{1}{6000}$	9.140670631721150	0.2192×10^{-2}

5. Conclusion

We have presented and compared different numerical approximations for the fractional derivative. The approximation based on the shifted Grünwald–Letnikov definition is the best option when considering first order approximations. For second order approximations, the approximation obtained from the Caputo definition performs better. Additionally precision problems related to the Lubich approximation are reported. These problems may be a consequence of the fact that we are unable to compute the weights with high accuracy.

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