Fourier Error Analysis of Caputo Derivative Approximations based on Lagrange Interpolation over Uniform Mesh

Shweta Kumari and Mani Mehra

Department of Mathematics, Indian Institute of Technology Delhi
New Delhi-110016, India
shwetakri8062@gmail.com, mmehra@maths.iitd.ac.in

Abstract. In this article, the modified wavenumbers for several numerical approximations of the Caputo fractional derivatives based on the Lagrange interpolation method over a uniform mesh are derived. With regard to the modified wavenumbers, the Fourier analysis of differencing errors is performed to quantify the resolution characteristics of these approximations. The plots of original wave numbers against modified wave numbers are presented for each approximation method. Numerical experiments over a test case are performed to validate the accuracy and efficiency of different approximation schemes for the Caputo fractional derivative.

Keywords: Caputo derivative · Fourier analysis of differencing errors · Modified wavenumbers · Resolution characteristics.

1 Introduction

The Caputo derivative is among the most prominent fractional derivatives studied in the field of fractional calculus. This is due to the non-local behavior and past memory containment of this derivative, which makes it favorable for modeling complex structured environmental phenomena. Furthermore, the Caputo derivative is important from the viewpoint of numerical interpretation of real-life problems, as the boundary conditions of the differential system remain analogous to the integer order system. Hence, various numerical algorithms are constructed in literature to approximate the Caputo derivative [8,5,15,16]. The $L1$ approach is the most popular approximation for the Caputo fractional derivative [13]. Lin and Xu [10] were the first to derive the classic $L1$ method for Caputo derivative approximation over a uniform mesh. The idea was to approximate the derivative in the integrand of the Caputo derivative expression by a linear interpolating polynomial in each of the time subintervals. This method had a convergence rate $\mathcal{O}(\tau^{2-\alpha})$. Following this idea with some upgradation, Gao et al. [4] proposed a new method with convergence of $\mathcal{O}(\tau^{3-\alpha})$ as the $L1$-2 method to approximate Caputo fractional derivative on a uniform mesh, where a linear and quadratic interpolation polynomial is used to discretize the integrand in first and other

ICCS Camera Ready Version 2025
To cite this paper please use the final published version:
DOI: 10.1007/978-3-031-97570-7_10

time subintervals, respectively. The latest addition is the $L1$-23 scheme of order $\mathcal{O}(\tau^{4-\alpha})$ developed for Caputo derivative approximation with an improvement of using cubic interpolating polynomials from the third subinterval onwards.

A classical technique to compare two difference schemes, other than the formal errors in numerical analysis, is Fourier analysis. It helps to analyse the dispersion and dissipation errors of the difference approximations by quantifying the resolution characteristics of the difference approximations. Numerous papers are dedicated to the Fourier error analysis of classical derivative approximations. Lele in [7] has discussed in detail the Fourier analysis of differencing errors for classical derivative approximations of first and second-order compact difference schemes. Authors in [12] have extended the study for higher-order classical derivative compact difference approximations. To study the Fourier error analysis of classical derivatives over a non-uniform mesh, see [1,3,11].

According to our best knowledge, [14] is the sole work that investigates the Fourier error analysis of fractional derivative approximations, in which the resolution characteristics of several difference approximations of Riemann-Liouville fractional derivative are investigated. As discussed, the Caputo fractional derivative is crucial in the analytical as well as numerical study of daily-life events. However, till now, no article is available in the literature on the Fourier error analysis of Caputo derivative approximations. Considering this as inspiration, we perform the Fourier error analysis of various numerical approximations of the Caputo fractional derivative based on Lagrange interpolation methods over a uniform mesh. In this process, the resolution formula for modified wavenumbers of difference approximations is derived.

The rest of the manuscript is organised as follows. In Section 2, some basic definitions and propositions are introduced concerning the Caputo fractional derivative and its numerical approximations based on methods of Lagrange interpolation over a uniform mesh. Section 3 is composed of the Fourier analysis of differencing errors of various Caputo derivative approximations introduced in the Preliminary section. The resolution formula for modified wavenumbers of the Caputo derivative and its approximations is obtained. To provide a basis for comparison and a better understanding of the work carried out, the Fourier error analysis of the finite difference approximation of the first-order derivative is presented first. This section also consists of the graphical comparison of the modified wavenumbers obtained versus the original wavenumber of the Caputo derivative and its approximations. The Final Section 5 provides the conclusion of this research with possible future directions.

2 Preliminaries

This section provides a foundation for this paper by introducing a few fundamental concepts related to the Caputo fractional derivative and its various approximations.

Definition 1. ***Caputo Derivative*** *[9]*
The left Caputo fractional derivative of order $\alpha > 0$ of the function $f(t)$, $t \in$

ICCS Camera Ready Version 2025
To cite this paper please use the final published version:
DOI: 10.1007/978-3-031-97570-7_10

(a, b), is defined as

$$ {}_C D_{a,t}^{\alpha} f(t) = \frac{1}{\Gamma(m-\alpha)} \int_a^t (t-s)^{m-\alpha-1} f^{(m)}(s) ds, $$

where $m - 1 < \alpha \leq m$, $m \in \mathbb{N}$. The left Caputo fractional derivative of $f(t)$ for a particular value of $m = 1$ such that $0 < \alpha < 1$ is

$$ {}_C D_{a,t}^{\alpha} f(t) = \frac{1}{\Gamma(1-\alpha)} \int_a^t (t-s)^{-\alpha} f'(s) ds. \tag{1} $$

Proposition 1. *[6] If $\mathrm{Re}(\alpha) > 0$ and $\lambda > 0$, then*

$$ ({}_C D_{+}^{\alpha} e^{\lambda t})(x) = \lambda^{\alpha} e^{\lambda x} \text{ and } ({}_C D_{-}^{\alpha} e^{-\lambda t})(x) = \lambda^{\alpha} e^{-\lambda x}. $$

Based on Lagrange interpolation methods, the following are some numerical approximations of the Caputo fractional derivative for $\alpha \in (0, 1)$.

Definition 2. *$L1$ **Method** [10]*
The $L1$ method for approximation of the Caputo fractional derivative is defined as

$$ {}_C D_{0,t}^{\alpha} f(t)\Big|_{t=t_j} = \frac{1}{\Gamma(1-\alpha)} \sum_{k=0}^{j-1} \frac{f(t_{k+1}) - f(t_k)}{\tau} \int_{t_k}^{t_{k+1}} (t_j - s)^{-\alpha} ds + \epsilon^j, \tag{2} $$

where τ is the step size, and $\epsilon^j = \mathcal{O}(\tau^{2-\alpha})$ is approximation error, provided $f(t) \in C^2[0, T]$.

Definition 3. *$L1$-2 **method** [4]*
The $L1$-2 method for approximation of the Caputo fractional derivative is defined as

$$ {}_C D_{0,t}^{\alpha} f(t)\Big|_{t=t_j} = \frac{\tau^{-\alpha}}{\Gamma(2-\alpha)} \left[c_0 f(t_j) - \sum_{n=1}^{j-1} (c_{j-n-1} - c_{j-n}) f(t_n) - c_{j-1} f(t_0) \right] + \epsilon^j, \tag{3} $$

where τ is the step size and the approximation error $\epsilon^j = \mathcal{O}(\tau^{3-\alpha})$, provided $f(t) \in C^3[0, T]$. Here $c_0 = a_0 = 1$ for $n = 1$; and for $n \geq 2$,

$$ c_n = \begin{cases} a_0 + b_0, & n = 0, \\ a_n + b_n - b_{n-1}, & 1 \leq n \leq j-2, \\ a_n - b_{n-1}, & n = j-1, \end{cases} $$

where

$$ a_n = (n+1)^{1-\alpha} - n^{1-\alpha}, \quad 0 \leq n \leq j-1. $$
$$ b_n = \left[(n+1)^{2-\alpha} - n^{2-\alpha}\right] / (2-\alpha) - \left[(n+1)^{1-\alpha} + n^{1-\alpha}\right] / 2, \quad n \geq 0. $$

ICCS Camera Ready Version 2025
To cite this paper please use the final published version:
DOI: 10.1007/978-3-031-97570-7_10

Definition 4. *$L1$-23 **method** [2]*
The $L1$-23 method for approximation of the Caputo fractional derivative is defined as

$$ {}_{C}D^{\alpha}_{0,t}f(t)\Big|_{t=t_j} = \frac{\tau^{-\alpha}}{\Gamma(2-\alpha)} \sum_{n=0}^{j} g_n f(t_{j-n}) + \epsilon^j, \tag{4} $$

where τ is the step size, and the approximation error $\epsilon^j = \mathcal{O}(\tau^{4-\alpha})$, provided $f(t) \in C^4[0,T]$. The coefficients $g_n s$ have the following values for different j:

$$
\begin{aligned}
&\textit{for } j=1,\; g_0 = a_0, \quad g_1 = -a_0;\\
&\textit{for } j=2,\; g_0 = a_0 + b_0, \quad g_1 = a_1 - a_0 - 2b_0, \quad g_2 = b_0 - a_1;\\
&\textit{for } j=3,\; g_0 = w_{1,0}, \quad g_1 = w_{2,0} + a_1 + b_1, \quad g_2 = w_{3,0} + a_2 - a_1 - 2b_1,\\
&\qquad g_3 = w_{4,0} - a_2 + b_1;\\
&\textit{for } j=4,\; g_0 = w_{1,0}, \quad g_1 = w_{1,1} + w_{2,0}, \quad g_2 = w_{2,1} + w_{3,0} + a_2 + b_2,\\
&\qquad g_3 = w_{3,1} + w_{4,0} + a_3 - a_2 - 2b_2, \quad g_4 = w_{4,1} - a_3 + b_2;\\
&\textit{for } j=5,\; g_0 = w_{1,0}, \quad g_1 = w_{1,1} + w_{2,0}, \quad g_2 = w_{1,2} + w_{2,1} + w_{3,0},\\
&\qquad g_3 = w_{2,2} + w_{3,1} + w_{4,0} + a_3 + b_3, \quad g_4 = w_{3,2} + w_{4,1} + a_4 - a_3 - 2b_3,\\
&\qquad g_5 = w_{4,2} - a_4 + b_3;\\
&\textit{for } 6 \le j \le J, \textit{ the relation between the coefficients takes form as follows:}\\
&\qquad g_0 = w_{1,0}, \quad g_1 = w_{1,1} + w_{2,0}, \quad g_2 = w_{1,2} + w_{2,1} + w_{3,0},\\
&\qquad g_n = w_{1,n} + w_{2,n-1} + w_{3,n-2} + w_{4,n-3}, \; (3 \le n \le j-3),\\
&\qquad g_{j-2} = a_{j-2} + b_{j-2} + w_{2,j-3} + w_{3,j-4} + w_{4,j-5},\\
&\qquad g_{j-1} = w_{3,j-3} + w_{4,j-4} + a_{j-1} + a_{j-2} + 2b_{j-2}, \quad g_j = w_{4,j-3} - a_{j-1}\\
&\qquad\qquad + b_{j-2},
\end{aligned}
$$

where

$$
\begin{aligned}
a_{j-2} &= (j-1)^{1-\alpha} - (j-2)^{1-\alpha},\\
b_{j-2} &= \frac{(j-1)^{2-\alpha} - (j-2)^{2-\alpha}}{2-\alpha} - \frac{(j-1)^{1-\alpha} + (j-2)^{1-\alpha}}{2},\\
w_{1,j-n} &= \frac{1}{6}\Big[2(j-n+1)^{(1-\alpha)} - 11(j-n)^{1-\alpha}\Big]\\
&\quad - \frac{1}{(2-\alpha)}\Big[2(j-n)^{2-\alpha} - (j-n+1)^{2-\alpha}\Big]\\
&\quad - \frac{1}{(2-\alpha)(3-\alpha)}\Big[(j-n)^{3-\alpha} - (j-n+1)^{3-\alpha}\Big],
\end{aligned}
$$

ICCS Camera Ready Version 2025
To cite this paper please use the final published version:
DOI: 10.1007/978-3-031-97570-7_10

$$
\begin{aligned}
w_{2,j-n} =& \frac{1}{2}\left[6(j-n)^{(1-\alpha)} + (j-n+1)^{1-\alpha}\right] \\
&+ \frac{1}{(2-\alpha)}\left[5(j-n)^{2-\alpha} - 2(j-n+1)^{2-\alpha}\right] \\
&- \frac{3}{(2-\alpha)(3-\alpha)}\left[(j-n)^{3-\alpha} - (j-n+1)^{3-\alpha}\right], \\
w_{3,j-n} =& -\frac{1}{2}\left[3(j-n)^{1-\alpha} + 2(j-n+1)^{1-\alpha}\right] \\
&- \frac{1}{2-\alpha}\left[4(j-n)^{2-\alpha} - (j-n+1)^{2-\alpha}\right] \\
&- \frac{3}{(2-\alpha)(3-\alpha)}\left[(j-n)^{3-\alpha} - (j-n+1)^{3-\alpha}\right], \\
w_{4,j-n} =& \frac{1}{6}\left[2(j-n)^{1-\alpha} + (j-n+1)^{1-\alpha}\right] + \frac{1}{2-\alpha}(j-n)^{2-\alpha} \\
&+ \frac{1}{(2-\alpha)(3-\alpha)}\left[(j-n)^{3-\alpha} - (j-n+1)^{3-\alpha}\right], \quad 3 \le n \le j.
\end{aligned}
$$

3 Fourier Error Analysis

In this section, the differencing errors, i.e., the dispersion and dissipation errors of various numerical approximations of Caputo fractional derivative, are obtained using the Fourier analysis approach. The approximations considered here for the Caputo fractional derivative are based on the method of Lagrange interpolation over a uniform mesh. This process of finding errors also quantifies the resolution characteristics of derivative approximations. First, the Fourier analysis of integer-order derivatives is discussed to provide a base for better understanding and comparison. Following that, the Fourier analysis of different approximations of the Caputo derivative based on Lagrange interpolation methods over a uniform mesh is established. To proceed with the analysis, the dependent variable $y(x)$ is assumed to be periodic over the domain $[0, L]$ of the independent variable x. Furthermore, the domain $[0, L]$ is discretized by choosing an even positive integer J such that $h = L/J$ is the stepsize of the grid domain. Hence, the Fourier series of $y(x)$ is written as

$$
y(x) = \sum_{k=-J/2}^{J/2} \hat{y}_k e^{\frac{2\pi i k x}{L}}, \quad i = \sqrt{-1},
$$

with Fourier coefficients $\hat{y}_k = \frac{1}{L}\int_0^L y(x) e^{-\frac{2\pi i k x}{L}} dx$. The wavenumber and coordinate in Fourier modes are scaled by $\omega_k = \frac{2\pi k h}{L}$ and $s = \frac{x}{h}$, respectively. Hence, the above Fourier expression can be rewritten as

$$
y(x(s)) = \sum_{k=-J/2}^{J/2} \hat{y}_k e^{i\omega_k s}. \tag{5}
$$

ICCS Camera Ready Version 2025
To cite this paper please use the final published version:
DOI: 10.1007/978-3-031-97570-7_10

In the first place, as discussed, the resolution characteristics of the exact first derivative are introduced. The exact first derivative of the above equation with respect to s supplies

$$y'(x(s)) = \sum_{k=-J/2}^{J/2} \hat{y'_k} e^{i\omega_k s} = \sum_{k=-J/2}^{J/2} i\omega_k \hat{y}_k e^{i\omega_k s},$$

which implies $\hat{y'_k} = i\omega_k \hat{y}_k$. Next consider a specific Fourier mode ω_k from (5) at $x = x_j$ as

$$y(x)\big|_{x=x_j} = \hat{y}_k e^{i\omega_k s_j}. \tag{6}$$

The second-order finite difference approximation of $y'(x)$ at $x = x_j$ is

$$y'_j = \frac{y_{j+1} - y_{j-1}}{2h}. \tag{7}$$

Then, the left-hand side of the above expression is

$$\frac{dy}{dx}\Big|_{x_j} = \frac{1}{h}\frac{dy}{ds}\Big|_{s_j} = \frac{1}{h}\hat{y}'_k e^{i\omega_k s_j}.$$

Also, substituting y_j from (6) in (7) gives the right-hand side expression as $\frac{\hat{y}_k e^{i\omega_k s_j}}{2h}(e^{i\omega_k} - e^{-i\omega_k})$. Hence, it implies that

$$\frac{\hat{y}'_k}{\hat{y}_k} = \sin(\omega).$$

Therefore, dropping the subscript k and comparing the Fourier coefficients of exact and approximate derivatives, the resolution characteristics are

$$\omega'_{ex}(\omega) = (i\omega),$$
$$\omega'_{app}(\omega) = \sin(\omega),$$

where ω' is the modified wavenumber of the first derivative. The dispersion and dissipation errors of the approximations are obtained from the differences between real parts of the wavenumber and modified wavenumbers $[\mathrm{Re}\,(\omega' - \omega)\,, \mathrm{Re}\,(\omega'' - \omega)]$ and the imaginary parts of the wavenumber and modified wavenumber $[\mathrm{Im}\,(\omega' - \omega)\,, \mathrm{Im}\,(\omega'' - \omega)]$, respectively [7].

3.1 Resolution characteristics of Caputo derivative and its approximations

Caputo fractional derivative:

The α-th order Caputo derivative of (5) with respect to s using (1) and proposition 1 provides a function

$$y^{\alpha}(x(s)) = \sum_{k=-J/2}^{J/2} \hat{y^{\alpha}_k} e^{i\omega_k s} = \sum_{k=-J/2}^{J/2} (i\omega_k)^{\alpha} \hat{y}_k e^{i\omega_k s},$$

ICCS Camera Ready Version 2025
To cite this paper please use the final published version:
DOI: 10.1007/978-3-031-97570-7_10

with exact Fourier coefficients

$$\hat{y_k^{\alpha}} = (i\omega_k)^{\alpha}\hat{y}_k. \tag{8}$$

Let the Fourier series for $y^{\alpha}(x)$ be also represented as

$${}_{C}D^{\alpha}_{0,s}y(x(s)) = y^{\alpha}(x(s)) = \sum_{k=-J/2}^{J/2} \hat{y}^{\alpha}_k e^{i\omega_k s}, \tag{9}$$

where $\hat{y}^{\alpha}_k$ is derived from various difference approximations.

Next, we present resolution characteristics for various difference approximations of the Caputo fractional derivative of order $0 < \alpha < 1$ based on methods of Lagrange interpolation over the uniform mesh.

<u>$L1$ approximation:</u>

From (2), the discrete fractional differential operator of the $L1$ approximation of the Caputo fractional derivative on $y(x)$ at grid point x_j is

$${}_{C}D^{\alpha}_{J}y_j = \frac{1}{\Gamma(1-\alpha)} \sum_{m=0}^{j-1} \frac{y_{m+1} - y_m}{h} \int_{x_m}^{x_{m+1}} (x_j - s)^{-\alpha} ds,$$

where

$${}_{C}D^{\alpha}_{J}y(x_j) = {}_{C}D^{\alpha}_{0,t}y(x)\Big|_{x=x_j} + \epsilon^j,$$

which can be rewritten as

$${}_{C}D^{\alpha}_{J}y_j = \frac{h^{-\alpha}}{\Gamma(2-\alpha)} \left[b^{\alpha}_1 y_j - b^{\alpha}_j y_0 + \sum_{n=1}^{j-1} (b^{\alpha}_{n+1} - b^{\alpha}_n) y_{j-n} \right], \tag{10}$$

where, $b^{\alpha}_n = n^{1-\alpha} - (n-1)^{1-\alpha}$.

Consider a specific Fourier mode ω_k at $x = x_j$ as (6). Then, using the chain rule of Caputo fractional differentiation and (9), we have

$${}_{C}D^{\alpha}_{0,x}y\big|_{x_j} = \frac{1}{h^{\alpha}}\ {}_{C}D^{\alpha}_{0,s}y\big|_{s_j} = \frac{1}{h^{\alpha}} \hat{y}^{\alpha}_k e^{i\omega_k s_j}. \tag{11}$$

Also substituting expression of y_j from (6) in (10),

$$\text{R.H.S.} = \frac{h^{-\alpha}\hat{y}_k}{\Gamma(2-\alpha)} \left[b^{\alpha}_1 e^{i\omega_k s_j} - b^{\alpha}_j e^{i\omega_k s_0} + \sum_{n=1}^{j-1} (b^{\alpha}_{n+1} - b^{\alpha}_n) e^{i\omega_k s_{j-n}} \right].$$

Hence, it implies

$$\frac{\hat{y}^{\alpha}_k}{\hat{y}_k} = \frac{1}{\Gamma(2-\alpha)} \left[b^{\alpha}_1 - b^{\alpha}_j e^{-i\omega_k s_j} + \sum_{n=1}^{j-1} (b^{\alpha}_{n+1} - b^{\alpha}_n) e^{-i\omega_k s_n} \right]. \tag{12}$$

ICCS Camera Ready Version 2025
To cite this paper please use the final published version:
DOI: 10.1007/978-3-031-97570-7_10

Now comparing (8) and (12) with dropped subscript k, we get

$$w^{\alpha}_{ex}(\omega) = (i\omega)^{\alpha}, \tag{13}$$

$$w^{\alpha}_{L1}(\omega) = \frac{1}{\Gamma(2-\alpha)}\left[b^{\alpha}_{1} - b^{\alpha}_{j}e^{-i\omega_k s_j} + \sum_{n=1}^{j-1}(b^{\alpha}_{n+1} - b^{\alpha}_{n})e^{-i\omega_k s_n}\right], \tag{14}$$

where (13) is the resolution characteristics of exact differentiation and (14) is the resolution formula of $L1$ approximation.

<u>**$L1-2$ approximation:**</u>

The discrete Caputo fractional derivative of function $y(x)$ at grid point x_j has the $L1-2$ approximation (3) as

$${}_{C}D^{\alpha}_{J}y_j = \frac{h^{-\alpha}}{\Gamma(2-\alpha)}\left[c_0 y_j - \sum_{n=1}^{j-1}\left(c_{j-n-1} - c_{j-n}\right)y_n - c_{j-1}y_0\right], \tag{15}$$

Again, considering a specific Fourier mode ω_k at $x = x_j$ as (6) and using (9), we arrive at (11). Thereafter replacing y_j in (15) from (6) yields,

$$\text{R.H.S.} = \frac{h^{-\alpha}\hat{y}_k}{\Gamma(2-\alpha)}\left[c_0 e^{i\omega_k s_j} - \sum_{n=1}^{j-1}\left(c_{j-n-1} - c_{j-n}\right)e^{i\omega_k s_n} - c_{j-1}e^{i\omega_k s_0}\right].$$

Hence, it implies

$$\frac{\hat{y}^{\alpha}_{k}}{\hat{y}_k} = \frac{1}{\Gamma(2-\alpha)}\left[c_0 - \sum_{n=1}^{j-1}\left(c_{j-n-1} - c_{j-n}\right)e^{i\omega_k s_{n-j}} - c_{j-1}e^{-i\omega_k s_j}\right]. \tag{16}$$

Now dropping subscript k in (16), we get the resolution formula as

$$w^{\alpha}_{L1-2}(\omega) = \frac{1}{\Gamma(2-\alpha)}\left[b^{\alpha}_{1} - b^{\alpha}_{j}e^{-i\omega_k s_j} + \sum_{n=1}^{j-1}(b^{\alpha}_{n+1} - b^{\alpha}_{n})e^{-i\omega_k s_n}\right]. \tag{17}$$

<u>**$L1-23$ approximation:**</u>

The discrete Caputo fractional derivative of function $y(x)$ at grid point x_j has the $L1-23$ approximation (4) as

$${}_{C}D^{\alpha}_{J}y_j = \frac{h^{-\alpha}}{\Gamma(2-\alpha)}\sum_{n=0}^{j} g_n y_{j-n}. \tag{18}$$

Proceeding similarly as in the above steps by considering a specific Fourier mode ω_k at $x = x_j$ as (6). Using (9), we arrive at (11). After that, replacing y_j in (18) from (6) provides with,

$$\text{R.H.S.} = \frac{h^{-\alpha}\hat{y}_k}{\Gamma(2-\alpha)}\sum_{n=0}^{j} g_n e^{i\omega_k s_{j-n}}.$$

ICCS Camera Ready Version 2025
To cite this paper please use the final published version:
DOI: 10.1007/978-3-031-97570-7_10

Hence, comparing both sides, we get

$$\frac{\hat{y}_k^\alpha}{\hat{y}_k} = \frac{1}{\Gamma(2-\alpha)} \sum_{n=0}^{j} g_n e^{-i\omega_k s_n}. \tag{19}$$

Thus, dropping the subscript k above gives the resolution characteristics as

$$w_{L1-23}^\alpha(\omega) = \frac{1}{\Gamma(2-\alpha)} \left[b_1^\alpha - b_j^\alpha e^{-i\omega_k s_j} + \sum_{n=1}^{j-1} (b_{n+1}^\alpha - b_n^\alpha) e^{-i\omega_k s_n} \right]. \tag{20}$$

From the above Fourier analysis of differencing errors, the wavenumbers (ω) and modified wavenumbers (ω') for Caputo derivative and its various approximations are obtained. The next presentation is a graphical illustration of these modified wavenumbers versus the original wavenumber. We have the modified wavenumber for exact Caputo differentiation as ω^α, and the values of modified wavenumbers of difference approximations are plotted to observe the best match in terms of resolution characteristics for different values of α. The resulting figures 1, 2, and 3 show that the $L1$-23 approximation for the Caputo fractional derivative exhibits the best resolution characteristics in comparison to other approximations. Another observation tells that this comparison is irrespective of the values of α and the number of mesh points J.

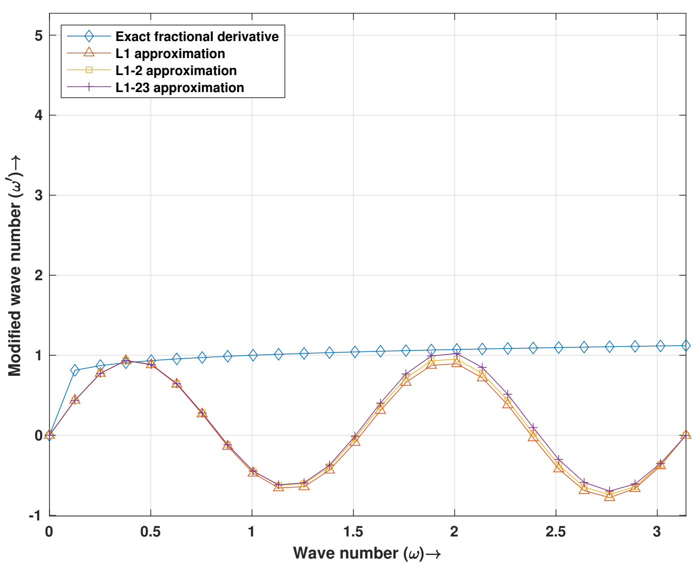

Fig. 1. Modified wavenumbers vs. wavenumber of difference approximations for $J = 50$ and $\alpha = 0.1$.

ICCS Camera Ready Version 2025
To cite this paper please use the final published version:
DOI: 10.1007/978-3-031-97570-7_10

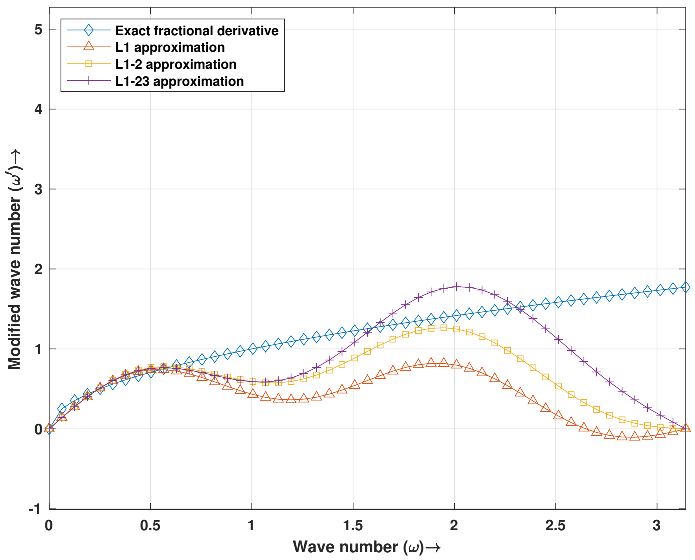

Fig. 2. Modified wavenumbers vs. wavenumber of difference approximations for $J = 100$ and $\alpha = 0.5$.

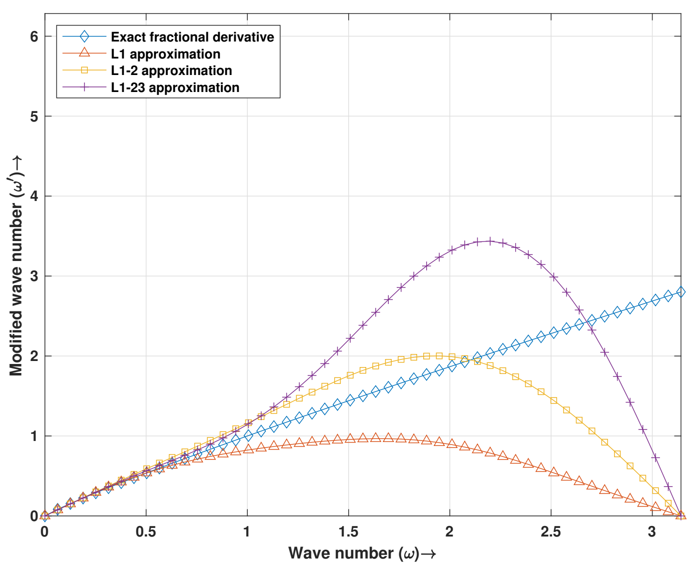

Fig. 3. Modified wavenumbers vs. wavenumber of difference approximations for $J = 100$ and $\alpha = 0.9$.

ICCS Camera Ready Version 2025
To cite this paper please use the final published version:
DOI: 10.1007/978-3-031-97570-7_10

4 Numerical Experiments

In this section, a few numerical experiments are performed on a test example of the Caputo fractional derivative initial value problem (IVP) by employing the Caputo derivative approximations studied in this work. The motive to conduct these experiments is to validate the accuracy of the approximations as well as characterise these approximations of the Caputo fractional derivative using various numerical parameters such as the step length of the interval and fractional order α. This study also provides the tradeoff between the computational costs and accuracy of the approximation schemes.

Example 1. Consider the following Caputo fractional derivative IVP:

$$\begin{aligned} {}_C D^{\alpha}_{0,t} y(t) &= \frac{t^3 \Gamma\left(4+\alpha\right)}{3!}, \quad t \in [0,1], \\ y(0) &= 0. \end{aligned}$$

It can be calculated that the exact solution to the above IVP is $y(t) = t^{3+\alpha}$. This IVP is a test case considering an α-dependent solution and with a zero initial condition.

Next, we employ $L1$, $L1$-2, and $L1$-23 from methods (2), (3) and (4) as Caputo derivative approximations in the above example and obtain the absolute error between the exact and numerical solution by varying the number of subintervals and values of α. The following formulas are used to obtain the absolute error and the corresponding rate of convergence.

$$E_{\infty}(N) = \left|e^N\right| = \left|y(t_N) - y^N\right|. \tag{21}$$

Thus, the convergence of error, using the error norm (21), in time, say T_{rate}, is defined as

$$T_{rate} = \log_2\left(\frac{E_{\infty}(N/2)}{E_{\infty}(N)}\right). \tag{22}$$

By the dint of various numerical experiments conducted over the test example 1, Table 1 represents the absolute errors and corresponding convergence rates of the $L1$ approximation scheme at final time $T = 1$ for different values of α and N. The tabular data clearly indicates the accuracy and efficiency of the scheme. As the value of α declines, there is a significant reduction in the absolute errors along with an explicit upsurge in the rate of convergence. The $L1$ scheme performs comparatively better for lower values of α and a higher number of subintervals and exhibits a convergence rate of $\mathcal{O}(\tau^{2-\alpha})$.

A similar set of numerical experiments is again performed over the test example 1 by approximating the Caputo fractional derivative with $L1$-2 and $L1$-23 approximation schemes, and the obtained results are displayed in Table 2 and 3, respectively. The displayed results showcase a similar pattern, where again the absolute errors are less for lower values of α and a higher number of subintervals. Thus, the convergence rates are also better for lower values of α. The

ICCS Camera Ready Version 2025
To cite this paper please use the final published version:
DOI: 10.1007/978-3-031-97570-7_10

Table 1. Absolute errors and order of convergence at $T = 1$ with $L1$ method.

N	$\alpha = 0.3$		$\alpha = 0.5$		$\alpha = 0.7$	
	E_∞	T_{rate}	E_∞	T_{rate}	E_∞	T_{rate}
10	1.3300e-02		3.5300e-02		7.7000e-02	
20	4.5000e-03	1.5634	1.3300e-02	1.4082	3.2400e-02	1.2489
40	1.5000e-03	1.5850	4.9000e-03	1.4406	1.3500e-02	1.2630
80	4.8019e-04	1.6433	1.8000e-03	1.4448	5.6000e-03	1.2695
160	1.5365e-04	1.6440	6.4474e-04	1.4812	2.3000e-03	1.2838
320	4.8741e-05	1.6564	2.3104e-04	1.4806	9.2967e-04	1.3068

$L1$-2 approximation scheme in Table 2 exhibits a convergence rate of $\mathcal{O}(\tau^{3-\alpha})$, whereas, in Table 3, the $L1$-23 approximation scheme displays a convergence rate of $\mathcal{O}(\tau^{4-\alpha})$. Hence, from the point of view of the accuracy of the approximation schemes for Caputo fractional derivative, the $L1$-23 scheme has a clear win.

Table 2. Absolute errors and order of convergence at $T = 1$ with $L1$-2 method.

N	$\alpha = 0.3$		$\alpha = 0.5$		$\alpha = 0.7$	
	E_∞	T_{rate}	E_∞	T_{rate}	E_∞	T_{rate}
10	3.0000e-03		8.6000e-03		1.9500e-02	
20	5.2955e-04	2.5021	1.7000e-03	2.3388	4.4000e-03	2.1479
40	8.8235e-05	2.5853	3.1793e-04	2.4188	9.4503e-04	2.2191
80	1.4341e-05	2.6212	5.8342e-05	2.4461	1.9775e-04	2.2567
160	2.2956e-06	2.6432	1.0553e-05	2.4669	4.0815e-05	2.2765
320	3.6380e-07	2.6577	1.8929e-06	2.4790	8.3623e-06	2.2871

Table 3. Absolute errors and order of convergence at $T = 1$ with $L1$-23 method.

N	$\alpha = 0.3$		$\alpha = 0.5$		$\alpha = 0.7$	
	E_∞	T_{rate}	E_∞	T_{rate}	E_∞	T_{rate}
10	3.7435e-04		1.3000e-03		3.5000e-03	
20	3.1120e-05	3.5885	1.2278e-04	3.4044	3.8548e-04	3.1826
40	2.5260e-06	3.6229	1.1365e-05	3.4334	4.1073e-05	3.2304
80	2.0195e-07	3.6448	1.0325e-06	3.4604	4.2783e-06	3.2631
160	1.5986e-08	3.6591	9.2812e-08	3.4757	4.4037e-07	3.2802
320	1.2566e-09	3.6692	8.2900e-09	3.4849	4.5040e-08	3.2894

However, when the total elapsed time taken in seconds to perform the simulation by all these difference approximations is calculated, we can see from Table 4 that the highest time is taken by the $L1$-23 approximation scheme.

ICCS Camera Ready Version 2025
To cite this paper please use the final published version:
DOI: 10.1007/978-3-031-97570-7_10

Table 4. Total elapsed time (in sec) at $\alpha = 0.5$ for different approximation schemes.

N	Elapsed time (in sec)		
	$L1$	$L1$-2	$L1$-23
10	0.009828	0.020611	0.037976
20	0.006573	0.026980	0.109275
40	0.005160	0.012928	0.041782
80	0.004253	0.012068	0.040428
160	0.005800	0.022178	0.092971
320	0.007439	0.065428	0.242998

5 Conclusion

This article provides a comparative analysis of differencing errors of various numerical approximations of the Caputo fractional derivative based on the methods of Lagrange interpolation over a uniform mesh. The resolution formula for modified wavenumbers of the Caputo derivative approximations is obtained using Fourier analysis and, thus, compares the differencing errors. The modified wavenumbers for these approximations are plotted against wavenumber ω for different values of α and J in Figs. 1, 2 and 3. From these figures, it is observed that the $L1-23$ approximation depicts better resolution characteristics as compared to other Caputo derivative approximations. Modification in fractional order α and/or the number of mesh points J does not influence the outcomes. Numerical simulations on a test case conducted using these approximations validate the accuracy of these schemes and showcase $L1$-23 as a better option for approximating the Caputo fractional derivative. Also, it confirms that these approximations perform better for lower values of α and a higher number of subintervals. One important aspect of Caputo derivative approximation based on Lagrange interpolation methods is the presence of an initial singularity of the function around $x = 0$, which deteriorates the scheme's convergence and is dealt with by considering a non-uniform mesh. Hence, we would like to extend this study to a comparative Fourier analysis of differencing errors of Caputo derivative approximations over the non-uniform mesh.

Acknowledgments. The research contributed by the first author in this paper is supported by the Council of Scientific and Industrial Research (CSIR), India, under grant number 09/086(1483)/2020-EMR-I.

Disclosure of Interests. The authors declare that they have no known and unknown competing interests that are relevant to the content of this article.

References

1. Cain, A., Bush, R.: Numerical wave propagation analysis for stretched grids. In: 32nd Aerospace Sciences Meeting and Exhibit. p. 172 (1994)

ICCS Camera Ready Version 2025
To cite this paper please use the final published version:
DOI: 10.1007/978-3-031-97570-7_10

2. Cao, J., Li, C., Chen, Y.: High-order approximation to Caputo derivatives and Caputo-type advection-diffusion equations (II). Fractional calculus and Applied analysis **18**(3), 735–761 (2015)
3. Gamet, L., Ducros, F., Nicoud, F., Poinsot, T.: Compact finite difference schemes on non-uniform meshes. Application to direct numerical simulations of compressible flows. International Journal for Numerical Methods in Fluids **29**(2), 159–191 (1999)
4. Gao, G.h., Sun, Z.z., Zhang, H.w.: A new fractional numerical differentiation formula to approximate the Caputo fractional derivative and its applications. Journal of Computational Physics **259**, 33–50 (2014)
5. Karatay, I., Kale, N., Bayramoglu, S.: A new difference scheme for time-fractional heat equations based on the Crank-Nicholson method. Fractional Calculus and Applied Analysis **16**(4), 892–910 (2013)
6. Kilbas, A.A., Srivastava, H.M., Trujillo, J.J.: Theory and applications of fractional differential equations, vol. 204. Elsevier (2006)
7. Lele, S.K.: Compact finite difference schemes with spectral-like resolution. Journal of Computational Physics **103**(1), 16–42 (1992)
8. Li, C., Chen, A., Ye, J.: Numerical approaches to fractional calculus and fractional ordinary differential equation. Journal of Computational Physics **230**(9), 3352–3368 (2011)
9. Li, C., Zeng, F.: Numerical methods for fractional calculus. CRC Press (2015)
10. Lin, Y., Xu, C.: Finite difference/spectral approximations for the time-fractional diffusion equation. Journal of Computational Physics **225**(2), 1533–1552 (2007)
11. Ma, Y., Gao, H., Fu, D., Li, X.: Difference schemes on non-uniform mesh and their application. Progress in Natural Science **14**(10), 848–854 (2004)
12. Mehra, M., Patel, K.S.: Algorithm 986: A suite of compact finite difference schemes. ACM Transactions on Mathematical Software (TOMS) **44**(2), 1–31 (2017)
13. Oldham, K., Spanier, J.: The fractional calculus theory and applications of differentiation and integration to arbitrary order, vol. 111. Elsevier (1974)
14. Patel, K.S., Mehra, M.: Fourth order compact scheme for space fractional advection–diffusion reaction equations with variable coefficients. Journal of Computational and Applied Mathematics **380**, 112963 (2020)
15. Sousa, E.: Numerical approximations for fractional diffusion equations via splines. Computers & Mathematics with Applications **62**(3), 938–944 (2011)
16. Sousa, E.: How to approximate the fractional derivative of order $1 < \alpha \leq 2$. International journal of bifurcation and chaos **22**(04), 1250075 (2012)

ICCS Camera Ready Version 2025
To cite this paper please use the final published version:
DOI: 10.1007/978-3-031-97570-7_10