Numerical Computation of Fractional Derivatives of Complex-Valued Analytic Functions

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Abstract

Highly accurate numerical approximations of analytic Caputo fractional derivatives are difficult to compute due to the upper bound singularity in its integral definition. However, it has been recently demonstrated that Caputo fractional derivatives of analytic functions can be numerically evaluated to double-precision accuracy by utilizing only function values in a grid. This is done by considering a modified Trapezoidal Rule (TR) and placing equispaced finite difference (FD) correction stencils at both endpoints. In terms of complex-valued analytic functions f(z), these fractional derivatives are multi-valued. In this paper, we provide several test functions for this numerical method of evaluating Caputo fractional derivatives. We produce figures of the principal branch of the functions' approximated fractional derivatives, and include error plots of these approximations.

Keywords: Fractional derivatives, finite differences, analytic functions, complex variables, contour integration.

1 Introduction

Fractional calculus is the extension of the differentiation D and integration I operators from integer orders to real and complex orders. Regarding differentiation of an analytic function f(z), derivatives of non-integer order at a point $z = z_0$ depend on every value of f

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along some curve joining z_0 and an evaluation point (rather than only on a small open neighborhood around z_0). These derivatives of arbitrary order are called fractional derivatives, and can be computed by integrating from a base point to an evaluation point.¹ Regarding the computation of fractional derivatives defined by integrals, the standard trapezoidal rule (TR) for numerical contour integration on grid-based function values fails to approximate fractional derivatives up to high-order accuracy. This is due to the singularity at the upper endpoint in the integrand of a fractional derivative as well as the endpoint weights of the TR in general. However, a recent modification to the TR has been shown to produce highly accurate convergence rates for fractional derivatives [5], capable of achieving double-precision 10^{-16} accuracy. In this paper, we utilize the method discussed in [5] to compute fractional derivatives of several complex-valued analytic functions with similar style illustrations as used in [4].

2 Mathematical background

In this section, we give a brief discussion of analytic functions, multi-valued functions, branch cuts, and the definition of the Caputo fractional derivative. We save the finite difference (FD) approximations for definite integrals and fractional derivatives for Sections 3 and 4, respectively, and then later apply it to produce figures of fractional derivatives of analytic functions in the following section.

2.1 Analytic functions

A complex-valued function f is an extension of real-valued functions in which complex numbers are mapped to complex numbers. If we write a complex number as z = x + iy with $x, y \in \mathbb{R}$ and $i^2 = -1$, then f(z) = u(x, y) + iv(x, y) where u(x, y) and v(x, y) are real-valued functions. We graph the real and imaginary parts separately, along with the magnitude |f(z)| and its corresponding phase portrait.

If f(z) is differentiable in an open neighborhood centered around $z = z_0$, then f(z) is analytic at z_0 if $f'(z_0) = \lim_{\Delta z \to 0} \frac{f(z_0 + \Delta z) - f(z_0)}{\Delta z}$ is uniquely defined at z_0 irrespective of direction by which $\Delta z \to 0$. If f is analytic, then it satisfies the Cauchy-Riemann (CR) equations

$$\frac{\partial u}{\partial x} = \frac{\partial v}{\partial y}, \qquad \frac{\partial u}{\partial y} = -\frac{\partial v}{\partial x}.$$
 (1)

Conversely, if f satisfies the CR equations, then f is analytic. There are numerous and significant consequences of the CR equations. Consequences include that f is infinitely differentiable and that it has a locally convergent Taylor series around z_0 . The common elementary functions are all analytic.⁴

¹Though they need not be defined by an integral [7].

⁴For more information on analytic functions, see for example [4].

2.2 Multi-valued functions and branch cuts

One property of fractional derivatives and of certain analytic functions is that they are multi-valued. A multi-valued function maps a single input value to several values. An example of a multi-valued function is $f(z) = \log(z)$. Taking z in polar coordinates and using the properties of logarithms yields $z = \log |z| + i\theta$. Since θ is 2π -periodic, f(z) = $\log |z| + i(\theta + 2\pi k)$, where $k \in \mathbb{Z}$. Thus, $\log(z)$ takes on infinitely many values for any z. Furthermore, z = 0 is a branch point singularity⁵ of $\log(z)$, i.e., a single loop around z = 0results in a different value from the starting point to the end point.

In order to make a multi-valued function single-valued, a branch cut must be chosen. A branch cut is a continuous curve from a branch point to another branch point in which a multi-valued function takes on a single-valued form, called a Riemann sheet. Although branch cuts can be chosen arbitrarily, the standard convention for a branch cut satisfies $\operatorname{Arg}(z) = \theta \in (-\pi, \pi]$, which places the branch cut from 0 to $-\infty$. Further illustrations and information on multi-valued functions and branch cuts can be found in chapter 2 of [4].

2.3 Fractional derivatives

In differential calculus, derivatives of integer order are local and tell us how a function f(z) behaves within a small neighborhood of function values around $z = z_0$. For derivatives of arbitrary order, known as *fractional derivatives*, this local property is not preserved, and hence fractional derivatives do not share all of the properties that integer-order derivatives possess. Related to this, many definitions of fractional derivatives exist, each of which aims to preserve some, but not all properties from integer order derivatives. Depending on the properties preserved from a defined fractional derivative, certain fractional derivatives can be more applicable than others. For this paper, we choose to focus on the Caputo fractional derivative:

$${}_{a}^{C}D_{t}^{\alpha}f(t) = \frac{1}{\Gamma(n-\alpha)} \int_{a}^{t} \frac{f^{(n)}(\tau)}{(t-\tau)^{\alpha+1-n}} d\tau, \qquad n-1 < \alpha < n,$$
(2)

which was first introduced by M. Caputo in [1]. The main preserving properties of the Caputo fractional derivative is that ${}_{0}D_{z}^{\alpha}(c) = 0$ for any constant c, and the Laplace Transform of a Caputo derivative can be expressed by the base-point values of f(t) and its integer-order derivatives,

$$\mathcal{L}\{{}_{0}^{C}D_{t}^{\alpha}f(t)\}(s) = s^{\alpha}F(s) - \sum_{k=0}^{n-1}s^{\alpha-k-1}f^{(k)}(0), \qquad n-1 < \alpha < n.$$
(3)

As a result, Caputo fractional derivatives are more favored for modeling initial value problems in fractional differential equations than other definitions of fractional derivatives [6, 7]. The main disadvantage of Caputo fractional derivatives over other fractional derivatives is that

⁵More specifically, a logarithmic singularity. Similarly, $z = \infty$ is also a logarithmic singularity.

 $f^{(n)}(t)$ must exist. In most cases however, $f^{(n)}(t)$ exists and is often assumed to exist when modeling fractional differential equations. In the case of complex-valued analytic functions f(z), $f^{(n)}(z)$ always exists and hence existence need not be verified.

Another fractional derivative definition is the Riemann-Liouville derivative:⁶

$${}_{0}^{RL}D_{t}^{\alpha}f(t) = \frac{1}{\Gamma(n-\alpha)}\frac{d^{n}}{dt^{n}}\int_{a}^{t}\frac{f(\tau)}{(t-\tau)^{\alpha+1-n}}d\tau, \qquad n-1 < \alpha < n.$$
(4)

One major similarity between the Caputo and Riemann-Liouville derivatives is that for any power function $f(t) = t^k$ with $k > \alpha$, its fractional derivative with a base point a = 0 is expressed as

$${}_{0}^{RL}D_{t}^{\alpha}f(t) = {}_{0}^{C}D_{t}^{\alpha}f(t) = \frac{\Gamma(k+1)}{\Gamma(k-\alpha+1)}t^{k-\alpha}.$$
(5)

Since analytic functions can be expressed as some locally convergent power series, it follows from (5) that fractional derivatives of analytic functions are multi-valued.⁷ As a result, we choose a branch cut such that the fractional derivative of some analytic function f(z) becomes single-valued. For this paper, we choose the standard branch cut.

Without loss of generality, we consider $0 < \alpha < 1$ and base point a = 0, (focusing first on t > 0, but later generalizing to any t), and introduce the notation ${}_{0}^{C}D_{t}^{\alpha} = D^{\alpha}$ for the remainder of the paper. Then (2) can be written as

$$D^{\alpha}f(t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{f'(\tau)}{(t-\tau)^{\alpha}} d\tau.$$
 (6)

We choose to consider $0 < \alpha < 1$ explicitly since $D^{\alpha+m}f(t) = D^{\alpha}f^{(m)}(t)$ for integer m, allowing us to extend this method to compute derivatives of any arbitrary order. In the case of approximating $D^{\alpha+m}f(t)$, the complex plane FD formulas discussed in [3] will suffice for computing $f^{(m)}(t)$. It should also be noted that the Caputo fractional derivative is non-commutative [6]. Furthermore, a = 0 is the standard convention for defining Caputo fractional derivatives [7].

3 FD approximation for definite integrals

One well-known method to approximate definite integrals is to use the trapezoidal rule (TR). The TR uses function values at N equispaced nodes located at $x_k = x_0 + kh$, for k = 0, 1, 2, ..., N, to obtain an approximate result of the form

$$\int_{x_0}^{x_N} f(x)dx \approx h \sum_{k=0}^N f(x_k) - \frac{h}{2} [f(x_0) + f(x_N)] + \mathcal{O}(h^2).$$
(7)

 $^{^{6}}$ Whose preserving properties and comparisons to the Caputo fractional derivative can be found in [6, 7], along with other definitions of fractional derivatives.

⁷Unless $f(z) = z^{k+\alpha}$ where k is an integer, thus producing a single-valued fractional derivative.

By the Euler-Maclaurin formula, the error between the exact integral value and the TR approximation becomes the following series:

$$\int_{x_0}^{x_N} f(x)dx - \text{TR} \approx \frac{h^2}{12} [f^{(1)}(x_0) - f^{(1)}(x_N)] - \frac{h^4}{720} [f^{(3)}(x_0) - f^{(3)}(x_N)] + \frac{h^6}{30240} [f^{(5)}(x_0) - f^{(5)}(x_N)] - \dots$$
(8)

One may also choose to numerically integrate a function with a midpoint expansion with nodes located at $x_k = x_0 + (k + \frac{1}{2})h$. In this case, the second Euler-Maclurin formula for this error expansion becomes

$$\int_{x_0}^{x_N} f(x)dx - \text{TR} \approx -\frac{h^2}{24} [f^{(1)}(x_0) - f^{(1)}(x_N)] + \frac{7h^4}{5760} [f^{(3)}(x_0) - f^{(3)}(x_N)] - \frac{31h^6}{967680} [f^{(5)}(x_0) - f^{(5)}(x_N)] + \cdots$$
(9)

The coefficients of (8) and (9) are extracted from the series expansions of $\frac{1}{1-e^{-z}} - \frac{1}{z}$ and $\frac{e^{z/2}}{e^z-1} - \frac{1}{z}$, respectively. In both cases, the majority of the error produced from utilizing the TR arises from the two endpoints.⁸ Thus, the weights at the endpoints should be adjusted to improve the accuracy.

One method to improve the accuracy of the TR is to place $N = (2n+1) \times (2n+1)$, $n = 1, 2, \ldots$, equispaced nodes of spacing h at both endpoints. These nodes, which are the FD correction stencils discussed in [2, 3], are used to create weights for the odd-ordered derivatives in the Euler-Maclurin formula. The accuracy of these FD stencils for the k^{th} derivative is $\mathcal{O}(h^{N-k})$. After creating as many FD stencils for the derivatives in the Euler-Maclurin formula are significant accuracy, these weights are then added up to create the final end correction stencils.

An example left-end correction stencil for odd-ordered derivatives up to $f^{(7)}(z)$ with 3×3 stencils for $\int_0^\infty f(x) dx$ is

$$\int_{0}^{\infty} f(x)dx \approx h \left\{ \begin{bmatrix} \frac{-821 - 779i}{403200} & -\frac{1889i}{100800} & \frac{821 - 779i}{403200} \\ -\frac{1511}{100800} & \frac{1}{2} & 1 + \frac{1511}{100800} \\ -\frac{821 + 779i}{403200} & \frac{1889i}{100800} & \frac{821 + 779i}{403200} \end{bmatrix} 1 1 1 1 1 \dots \right\}, (10)$$

where the boxed values are the added FD stencils. In the case of integrating on a finite interval, the right-end correction stencils are the negative of the left-end stencils. In either

⁸In the case that $f^{(n)}(z_0) = f^{(n)}(z_N)$ for positive odd integers *n*, the TR accuracy becomes highly accurate, as is the case for periodic functions.

case, the accuracy of the TR with 3×3 end-correction stencils is now increased to $\mathcal{O}(h^{10})$.

4 FD approximation for fractional derivatives

As discussed in [5], the two main issues with applying a TR-based approximation of the integral $I = \frac{1}{\Gamma(1-\alpha)} \int_0^z \frac{f'(\tau)}{(z-\tau)^{\alpha}} d\tau$ are the singularity created by $\frac{1}{(z-\tau)^{\alpha}}$ at the upper bound of the integrand, and the $f'(\tau)$ factor in the numerator of the integrand (as $f'(\tau)$ may not be numerically available). To fix these issues, we first split the interval [0, z] into [0, z - h] and [z - h, z], and then perform integration by parts on the first sub-interval. Excluding the $\frac{1}{\Gamma(1-\alpha)}$ constant, we obtain

$$I = \underbrace{\left\{-\frac{f(0)}{z^{\alpha}}\right\}}_{\text{left end}} \underbrace{-\alpha \left\{\int_{0}^{z-h} \frac{f(\tau)}{(z-\tau)^{\alpha+1}} d\tau\right\}}_{\text{central part}} + \underbrace{\left\{\frac{f(z-h)}{h^{\alpha}} + \int_{z-h}^{z} \frac{f'(\tau)}{(z-\tau)^{\alpha+1}} d\tau\right\}}_{\text{right end}}.$$
 (11)

By applying the TR to the central part of (11), we obtain

$$\int_0^{z-h} \frac{f(\tau)}{(z-\tau)^{\alpha+1}} d\tau \approx h \sum_{k=1}^{\left\lfloor \frac{z}{h} \right\rfloor - 1} \frac{f(kh)}{(z-kh)^{\alpha+1}}$$
(12)

The correction weights for each of these parts are derived in Section 3 of [5], where a change of variable $z - \tau = \sigma$ with $f(\tau) = f(z - \sigma) = c(\sigma)$ is performed on the singular parts of the central and right end parts of (11). From here, each correction weight follows a similar derivation of (10) obtained from [2]. Example $N = 5 \times 5$ singular part end correction weights for $\alpha = 0.5$ are given as

Using $N = 5 \times 5$ correction weights with $\alpha = 0.5$ increases the accuracy of the modified TR to $\mathcal{O}(h^{45/2})$ [5]. To evaluate at any arbitrary complex evaluation point z (rather than only at positive real z), piecewise linear paths are followed with rotated correction stencils that depend on the direction of the line of integration. Paths are also chosen such that no base point or corner point correction stencil is near the singular evaluation point. If the evaluation point is close to the base point, a Taylor expansion of f(z) centered at the midpoint between the base and evaluation point is evaluated numerically term by term to produce the same accuracy as the surrounding region. Further discussion of the paths followed from the base point to the evaluation point are described in Sections 4 and 5 of [5], with further special cases in Section 6.

5 Fractional derivatives of analytic functions

In this section, we test the FD method for fractional derivatives discussed in [5] on a collection of analytic functions for different α using MATLAB. Since most analytic functions do not have an exact solution for their Caputo fractional derivatives, we have selected test cases where exact results can be found in [8] or by Mathematica. Some of the fractional derivatives are represented by $_{3}F_{2}$ hypergeometric functions, which produce an excessively long computation time for testing the relative error of some functions. To speed up this computation time, the $_{3}F_{2}$ function values are evaluated on a grid in Mathematica, and then transferred to MATLAB to test the relative error. From this method, figures 11 - 14 appear to produce a large error around the unit circle. This is believed to occur due to how Mathematica computes the generalized $_{p}F_{q}$ hypergeometric functions and not caused by the present algorithm. Larger errors near the logarithmic singularities are also present, but expected.

For these test functions, we compute the real and imaginary parts, the complex magnitude with its corresponding color wheel, and a relative error plot at each node. Each of these figures use a square domain containing 70 nodes along the real and imaginary axes with a step size of $h = \frac{1}{20}$ to produce a square 3.5×3.5 domain centered around z = 0. We also choose to use $N = 5 \times 5$ correction stencils around the base and evaluation points to produce double-precision accuracy with this FD method.⁹ In the real and imaginary parts, the red curve represents when y = 0, and the black curve in the complex magnitude plot also represents when y = 0. In the error plot, the red circle indicates the region in which the midpoint Taylor expansion method is used. We further choose to restrict these functions on small domains to show where these branch cuts restrict these multi-valued functions into single-valued functions.

⁹With an accuracy of $\mathcal{O}(h^{45/2})$ for $\alpha = 0.5$, it is possible to achieve higher precision accuracy using one of MATLAB's extended precision toolboxes.



Figure 1: FD approximation of $D^{\alpha}e^{-z^2}$ with $\alpha = \frac{1}{3}$ whose analytic Caputo α -derivative is $-\frac{9z^{5/3}}{5\Gamma(2/3)} {}_2F_2(1, \frac{3}{2}; \frac{4}{3}, \frac{11}{6}; -z^2).$



Figure 2: FD approximation of $D^{\alpha} \log(1+z)$ with $\alpha = \frac{1}{2}$ whose analytic Caputo α -derivative is $\frac{2 \operatorname{arcsinh}(\sqrt{z})}{\sqrt{\pi(1+z)}}$.



Figure 3: FD approximation of $D^{\alpha} \sin(\pi z)$ with $\alpha = \frac{\pi}{8}$ whose analytic Caputo α -derivative is $\frac{\pi z^{1-\pi/8}}{\Gamma(1-\pi/8)} {}_1F_2(1; 1-\frac{\pi}{8}, \frac{3}{2}-\frac{\pi}{16}; -\frac{\pi^2 z^2}{4}).$



Figure 4: FD approximation of $D^{\alpha} \cos\left(\frac{\pi}{2}z\right)$ with $\alpha = \frac{\pi}{4}$ whose analytic Caputo α -derivative is $-\frac{\pi^2 z^{2-\pi/4}}{4\Gamma(1-\pi/4)} {}_1F_2(1; \frac{3}{2} - \frac{\pi}{8}, 2 - \frac{\pi}{8}, -\frac{\pi^2 z^2}{16}).$



Figure 5: FD approximation of $D^{\alpha} \sinh(z)$ with $\alpha = \frac{1}{5}$ whose analytic Caputo α -derivative is $\frac{5z^{4/5}}{4\Gamma(4/5)} {}_1F_2(1; \frac{9}{10}, \frac{7}{5}, \frac{z^2}{4})$.



Figure 6: FD approximation of $D^{\alpha} \cosh(z)$ with $\alpha = \frac{2}{5}$ whose analytic Caputo α -derivative is $\frac{25z^{8/5}}{24\Gamma(3/5)} {}_1F_2(1; \frac{9}{10}, \frac{7}{5}; \frac{z^2}{4})$.



Figure 7: FD approximation of D^{α} fresnel C(z) with $\alpha = \frac{3}{5}$ whose analytic Caputo α -derivative is $\frac{5z^{2/5}}{2\Gamma(2/5)} {}_{3}F_{4}(\frac{1}{4}, \frac{3}{4}, 1; \frac{7}{20}, \frac{3}{5}, \frac{17}{20}, \frac{11}{10}; -\frac{\pi^{2}z^{4}}{16}).$



Figure 8: FD approximation of D^{α} freshels(z) with $\alpha = \frac{4}{5}$ whose analytic Caputo α -derivative is $\frac{125\pi z^{11/5}}{66\Gamma(1/5)} {}_{3}F_{4}(\frac{3}{4}, 1, \frac{5}{4}; \frac{4}{5}, \frac{21}{20}, \frac{13}{10}, \frac{31}{20}; -\frac{\pi^{2}z^{4}}{16}).$



Figure 9: FD approximation of $D^{\alpha}J_1(z)$ with $\alpha = \frac{2}{3}$ whose analytic Caputo α -derivative is $\frac{4}{27\Gamma(7/3)z^{5/3}} \left(2_1F_2(-\frac{1}{2};-\frac{1}{3},\frac{1}{6};-\frac{z^2}{4}) + 9z^2 {}_1F_2(\frac{1}{2};\frac{2}{3},\frac{7}{6};-\frac{z^2}{4}) - 2 \right).$



Figure 10: FD approximation of $D^{\alpha} \operatorname{erf}(z)$ with $\alpha = \frac{1}{2}$ whose analytic Caputo α -derivative is $\frac{4\sqrt{z}}{\pi} {}_{2}F_{2}(\frac{1}{2}, 1; \frac{3}{4}, \frac{5}{4}; -z^{2}).$



Figure 11: FD approximation of $D^{\alpha} \arcsin(z)$ with $\alpha = \frac{3}{4}$ whose analytic Caputo α -derivative is $\frac{4z^{1/4}}{\Gamma(1/4)} {}_{3}F_{2}(\frac{1}{2}, \frac{1}{2}, 1; \frac{5}{8}, \frac{9}{8}; z^{2}).$



Figure 12: FD approximation of $D^{\alpha} \arccos(z)$ with $\alpha = \frac{1}{4}$ whose analytic Caputo α -derivative is $-\frac{4z^{3/4}}{3\Gamma(3/4)} {}_{3}F_{2}(\frac{1}{2}, \frac{1}{2}, 1; \frac{7}{8}, \frac{11}{8}; z^{2}).$



Figure 13: FD approximation of $D^{\alpha} \arctan(z)$ with $\alpha = \frac{13}{20}$ whose analytic Caputo α -derivative is $\frac{20z^{7/20}}{7\Gamma(7/20)} {}_{3}F_{2}(\frac{1}{2}, 1, 1; \frac{27}{40}, \frac{47}{40}; -z^{2}).$



Figure 14: FD approximation of $D^{\alpha} \operatorname{arctanh}(z)$ with $\alpha = \frac{7}{20}$ whose analytic Caputo α -derivative is $\frac{20z^{13/20}}{13\Gamma(13/20)} {}_{3}F_{2}(\frac{1}{2}, 1, 1; \frac{33}{40}, \frac{53}{40}; z^{2}).$

6 Conclusion

By using the FD-based TR method discussed in [5], numerous tests of Caputo fractional derivatives of complex-valued analytic functions have here been approximated with near double-precision accuracy. Since this method has successfully approximated a large number of Caputo fractional derivatives, we can now produce figures of presently unknown fractional derivatives of analytic functions.¹⁰ As a result, future work may include determining approximate solutions to unknown fractional derivatives. It may also be of interest to approximate fractional derivatives on several Riemann sheets, including how many Riemann sheets a derivative of order α produces for a given function f(z). It may also be possible to generalize α to complex numbers to produce approximate complex-ordered fractional derivatives of analytic functions.

7 Acknowledgements

The author would like to thank Cécile Piret for providing most of the code used to produce the figures presented in this paper. The author would also like to thank Bengt Fornberg for his helpful advice throughout this project.

References

- M. Caputo, Linear model of dissipation whose Q is almost frequency independent II, Geophys. J.R. Astr. Soc. 13 (1967), 529-539.
- B. Fornberg, Contour integrals of analytic functions given on a grid in the complex plane, IMA Journal of Numerical Analysis 41 (2021), 814-825.
- [3] B. Fornberg. Finite difference formulas in the complex plane, Numerical Algorithms 90 (2022), 1305-1326.
- [4] B. Fornberg and C. Piret, Complex Variables and Analytic Functions: An Illustrated Introduction, SIAM, Philadelphia, 2020.
- [5] B. Fornberg and C. Piret, Computation of fractional derivatives of analytic functions, (2022), work in progress
- [6] M.K. Ishteva, *Properties and applications of the Caputo fractional operator*, Master's thesis, University of Karlsruhe, 2005.
- [7] I. Podlubny, Fractional Differential Equations, Academic Press, 1990
- [8] G. Scheidrin, N. C. Smith, A. Gladkina, and L. D. Carr, Exact results for a fractional derivative of elementary functions, SciPost Phys. 4 (2018).

¹⁰Or rather, fractional derivatives that cannot be computed using Mathematica's current algorithms.