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A new fractional numerical differentiation formula to approximate the Caputo fractional derivative and its applications ☆

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ABSTRACT

In the present work, first, a new fractional numerical differentiation formula (called the *L1-2 formula*) to approximate the Caputo fractional derivative of order α $(0<\alpha<1)$ is developed. It is established by means of the quadratic interpolation approximation using three points $(t_{j-2}, f(t_{j-2}))$, $(t_{j-1}, f(t_{j-1}))$ and $(t_j, f(t_j))$ for the integrand $f(t)$ on each small interval $[t_{j-1}, t_j]$ $(j \geqslant 2)$, while the linear interpolation approximation is applied on the first small interval $[t_0, t_1]$. As a result, the new formula can be formally viewed as a modification of the classical *L1 formula*, which is obtained by the piecewise linear approximation for $f(t)$. Both the computational efficiency and numerical accuracy of the new formula are superior to that of the *L1 formula*. The coefficients and truncation errors of this formula are discussed in detail. Two test examples show the numerical accuracy of *L1-2 formula*. Second, by the new formula, two improved finite difference schemes with high order accuracy in time for solving the time-fractional sub-diffusion equations on a bounded spatial domain and on an unbounded spatial domain are constructed, respectively. In addition, the application of the new formula into solving fractional ordinary differential equations is also presented. Several numerical examples are computed. The comparison with the corresponding results of finite difference methods by the *L1 formula* demonstrates that the new *L1-2 formula* is much more effective and more accurate than the *L1 formula* when solving time-fractional differential equations numerically.

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1. Introduction

In recent years, the fractional calculus has gained a great development in both theory and application. Its appearance and development, to a certain extent, make up for defects of the classical calculus of integer order. The fractional calculus has been used to describe many phenomenons in almost all applied sciences, such as fluid flow in porous materials, anomalous diffusion transport, acoustic wave propagation in viscoelastic materials, dynamics in self-similar structures, signal processing, financial theory, electric conductance of biological systems and others (see [1–5]).

As we know, the fractional derivatives have several different kinds of definitions, among which the Riemann–Liouville fractional derivative and the Caputo fractional derivative are two of the most important ones in applications [6]. The Risez

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fractional derivative is a linear representation of the left Riemann–Liouville fractional derivative and right Riemann–Liouville fractional derivative. A close relationship exists between the Riemann–Liouville fractional derivative and the Caputo fractional derivative. The Riemann–Liouville fractional derivative can be converted to the Caputo fractional derivative under some regularity assumptions of the function [2,6]. In fractional partial differential equations, the time-fractional derivatives are commonly defined using the Caputo fractional derivatives. The main reason lies in that the Riemann–Liouville approach needs initial conditions containing the limit values of Riemann–Liouville fractional derivative at the origin of time $t = 0$, whose physical meanings are not very clear. However, in cases with the time-fractional Caputo derivative, the initial conditions take the same form as that for integer-order differential equations, namely, the initial values of integer-order derivatives of functions at the origin of time $t = 0$ [2,6,7].

Until now, amounts of differential equations involving the fractional derivatives have emerged. Many literatures explored analytical solutions using the Laplace transform, Fourier transform, Mellin transform, method of variable separation and other techniques [2,8]. However, the exact analytical solutions are only known for a few simple cases and refer to some special functions such as the Fox *H* function and the hyperbolic geometry function [2,8]. The complexity of computing these special functions and the difficulties of finding exact solutions for most problems limit the applications of powerful fractional differential equations in engineering and scientific computing fields. Many scholars are devoting to the numerical algorithm of fractional differential equations, including the finite difference method, finite element method, and spectral element method [9–22], among which, the finite difference method is especially favored due to its simplicity in both calculation and analysis.

The fractional numerical differentiation formula is by itself important for research. Furthermore, it is also necessary for solving the numerical solutions of fractional differential equations. The Grünwald–Letnikov (*GL*) formula and the *L1 formula* are two major numerical differentiation formulae to directly discretize fractional derivatives. For the fractional derivative of order α $(0 < \alpha < 1)$, the *GL formula* usually can only get the first-order accuracy [2,9–13] and the *L1 formula* can achieve an improved accuracy of order $2 - \alpha$ [14–20]. In fact, the *L1 formula* is established by a piecewise linear interpolation approximation for the integrand function on each small interval. A natural idea is to apply a higher-order interpolation instead of the linear interpolation to improve the numerical accuracy. This is the initial motivation of our present work. Odibat [23] presented an algorithm to numerically approximate the fractional integration and Caputo fractional differentiation, where a modified trapezoidal rule is used and the Caputo fractional differentiation is approximated by a weighted sum of the ordinary derivatives of functions. Li, Chen and Ye [24] proposed some high-order numerical approximations for fractional integrals based on cubic Hermite interpolation and cubic spline interpolation and established several numerical algorithms to approximate the Caputo fractional derivatives by the quadratic interpolation. The starting point of the latter one was based on the equivalent integral form of the original differential system. The similar idea was applied by Cao and Xu [25] to approximate fractional ordinary differential equations (ODEs), where the so-called block-by-block approach was used and the unknown solutions were coupled in the first two steps. Our work here is aimed to directly discretize the fractional derivative instead of transforming the corresponding differential equation into its integral form. An explicit high-order numerical differentiation formula for the Caputo fractional derivative will be established and it can be applied into numerically solving fractional differential equations.

The plan of the remainder is as follows. In Section 2, a new fractional numerical differentiation formula (*L1-2 formula*) for the Caputo fractional derivative of order α $(0 < \alpha < 1)$ is derived. And the coefficient properties together with truncation error analysis of the formula are given. Two test examples are used to confirm convergence orders of the new formula in Section 3. In Section 4, we apply the new *L1-2 formula* to solve a class of fractional sub-diffusion equations on a bounded spatial domain and on an unbounded spatial domain, respectively. The computational results are compared with the corresponding ones with the *L1 formula*. Moreover, the application of the new *L1-2 formula* into solving fractional ODEs is also given. Finally, a brief conclusion and the further work have been listed.

2. Derivation of the new fractional numerical differentiation formula (*L1-2 formula*)

In this section, we mainly describe the process of deriving the new fractional numerical differentiation formula. Denote $t_k = k\Delta t$, $t_{k+\frac{1}{2}} = (t_{k+1} + t_k)/2$, $k \geqslant 0$, where Δt is the temporal step length. Introduce the following difference quotient operators:

$$\delta_t f_{k-\frac{1}{2}} = \frac{f(t_k) - f(t_{k-1})}{\Delta t}, \qquad \delta_t^2 f_k = \frac{1}{\Delta t}(\delta_t f_{k+\frac{1}{2}} - \delta_t f_{k-\frac{1}{2}}), \quad k \geqslant 1.$$

Suppose $f(t) \in C^1[0, t_k]$ $(k \geqslant 0)$. From the definition of the Caputo fractional derivative, we know that for any α $(0 < \alpha < 1)$

$$ {}_0^C\mathcal{D}_t^\alpha f(t)|_{t=t_k} = \frac{1}{\Gamma(1-\alpha)} \int_0^{t_k} \frac{f'(s)}{(t_k - s)^\alpha}\, \mathrm{d}s = \frac{1}{\Gamma(1-\alpha)} \sum_{j=1}^{k} \int_{t_{j-1}}^{t_j} \frac{f'(s)}{(t_k - s)^\alpha}\, \mathrm{d}s. \tag{2.1}$$

On each small interval $[t_{j-1}, t_j]$ $(1 \leqslant j \leqslant k)$, denoting the linear interpolation function of $f(t)$ as $\Pi_{1,j} f(t)$, i.e.,

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