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Second-order approximations for variable order fractional derivatives: Algorithms and applications

Xuan Zhao [a,*], Zhi-zhong Sun [a], George Em Karniadakis [b]

[a] Department of Mathematics, Southeast University, Nanjing 210096, People's Republic of China
[b] Division of Applied Mathematics, Brown University, Providence, RI 02912, USA

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ABSTRACT

Fractional calculus allows variable-order of fractional operators, which can be exploited in diverse physical and biological applications where rates of change of the quantity of interest may depend on space and/or time. In this paper, we derive two second-order approximation formulas for the variable-order fractional time derivatives involved in anomalous diffusion and wave propagation. We then present numerical tests that verify the theoretical estimates of convergence rate and also simulations of anomalous sub-diffusion and super-diffusion that demonstrate new localized diffusion rates that depend on the curvature of the variable-order function. Finally, we perform simulations of wave propagation in a truncated domain to demonstrate how erroneous wave reflections at the boundaries can be eliminated by super-diffusion, and also simulations of the Burgers equation that serve as a testbed for studying the loss and recovery of monotonicity using again variable rate diffusion as a function of space and/or time. Taken together, our results demonstrate that variable-order fractional derivatives can be used to model the physics of anomalous transport with spatiotemporal variability but also as new effective numerical tools that can deal with the long-standing issues of outflow boundary conditions and monotonicity of integer-order PDEs.

1. Introduction

Fractional calculus allows integration and differentiation at any fractional order [1–3], and moreover the order of fractional integration and differentiation can be a function of space and/or time. Samko and Ross [4] and Samko [5] generalized the Riemann–Liouvile and Marchaud fractional integration and differentiation for the case of variable-order and they presented interesting properties and an inversion formula. Lorenzo and Hartley [6] presented the concept of variable-order (VO) operators and investigated several potential variable-order definitions. In fact, even before the introduction of this new concept there were a few applications towards it. Smit and deVries [7] studied the stress–strain behavior of viscoelastic materials (textile fibers) with fractional order differential equations of order α $(0 \le \alpha \le 1)$ and showed that α depends on the strain level. Bagley [8] investigated the polymer linear viscoelastic stress relaxation described by fractional differential equations of order β for a given fixed temperature. This paper reveals a clear dependence of β on the temperature for polyisobutlene and correlates fractional models and experiments. In addition, Metzler et al. [9] found that the order of fractional

* Corresponding author.
E-mail addresses: xuanzhao11@gmail.com (X. Zhao), zzsun@seu.edu.cn (Z.-z. Sun), george_karniadakis@brown.edu (G.E. Karniadakis).

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derivative of the fractional partial differential equations (FPDEs) describing the relaxation processes and reaction kinetics of proteins depends on temperature.

There have been several other applications with variable-order models. Ingman et al. [10] demonstrated the effectiveness of using a dynamic integro-differential operator of variable-order for cases of viscoelastic and elastoplastic spherical indentation. Furthermore, the dependence of the order function on the strain and strain rate of viscoelastic material was evaluated in [14]. Later, Lorenzo and Hartley [11] explored more deeply the concept of VO integration and differentiation and created meaningful definitions for VO integration and differentiation. They also presented two forms of order distributions with applications to dynamic processes. Coimbra [12] and Diaz and Coimbra [17] investigated the dynamics and control of a nonlinear viscoelasticity oscillator via VO operators. Kobelev et al. investigated statistical and dynamical systems with fixed and variable memories, with the fractal dimension of the system being variable with time and spatial coordinate [13]. Pedro et al. studied the motion of particles suspended in a viscous fluid with drag force determined using the VO calculus [15]. Sun et al. [16] discussed four variable-order differential operators in anomalous diffusion modeling. They concluded that these four models, i.e., time/space/concentration/system parameter dependent VO models are more suitable in simulating the generalized decelerating/accelerating diffusion processes than the constant order model.

Gerasimov et al. [18] considered problems of anomalous infiltration in porous media. They proposed a fractional diffusion equation with variable-order of the time-derivative operator for describing the liquid infiltration in porous media according to the experimental data. They showed that the modified model with time fractional order depending on the concentration provides good agreement with existing experimental data for both the sub-diffusion and the super-diffusion. Sun et al. [19] analyzed mean square displacement (MSD) for characterizing anomalous diffusion and proposed an approach to establish a variable-random-order model for a given MSD function. Sun et al. [20] provided comparisons of constant-order and VO fractional models in characterizing the memory property of different systems. The advantages and potential applications of two variable-order derivative definitions were highlighted through a comparative analysis of anomalous relaxation process. Sun et al. [21] proposed a variable-index fractional-derivative model to describe the underlying transport dynamics.

The variable-order operator definitions recently proposed in the literature include the Riemann–Liouvile definition, Caputo definition, Marchaud definition, Coimbra definition and Grünwald definition. However, Soon et al. [22] also showed that the Coimbra definition variable-order operator satisfies a mapping requirement, and it is the only definition that correctly describes position-dependent transitions between elastic and viscous regimes because it correctly returns the appropriate derivatives as a function of space and time. Ramirez and Coimbra [23] showed that the Coimbra definition is the most appropriate definition having fundamental characteristics that are desirable for physical modeling.

Since the kernel of the variable-order operators has a variable-exponent, analytical solutions to variable-order fractional differential equations are more difficult to obtain. The solutions of the VO models are defined in fractional Besov spaces of variable-order on $\mathbb{R}^n$ [24]. Lin et al. [25] constructed an explicit finite difference scheme for spatial VO fractional differential equation, in which the space derivative is a generalized Riesz fractional derivative of order $\alpha(x,t)$ $(1 < \alpha(x,t) \le 2)$, where x and t are space and time variables, respectively, and they demonstrated stability and convergence of their scheme. The convergence order is one for both time and space. In a series of papers Chen et al. [26–28] studied various variable-order PDEs. Specifically, in [26], they proposed a numerical scheme with first-order temporal accuracy and fourth-order spatial accuracy for the VO anomalous sub-diffusion equation. The convergence, stability, and solvability of the numerical scheme were shown via Fourier analysis. In [27], they investigated the finite difference method for the variable-order nonlinear Stokes' first problem for a heated generalized second grade fluid. In [28], they considered the numerical method for a variable-order nonlinear reaction-subdiffusion equation and analyzed its stability and convergence. Recently, Chen et al. [29] proposed an alternating direct implicit method for a new two-dimensional variable-order fractional percolation equation with variable coefficients.

In [30], Valério and Sá da Costa addressed the different possible definitions of VO derivatives and their numerical approximations. Sun et al. [31] developed three finite difference schemes for VO fractional sub-diffusion equation (VOFSE) with time fractional order $\alpha(x,t)$ $(0 < \alpha(x,t) < 1)$. They showed that all the schemes have first-order temporal accuracy and second-order spatial accuracy. Shen et al. [32] also studied VOFSE and proposed a finite difference scheme with accuracy $O(\tau + h^2)$. Chen et al. [33] presented an implicit scheme for solving VOFSE in two-dimensions. The scheme was proved to be convergent with order $O(\Delta_t + \Delta_x^2 + \Delta_y^2)$, where Δ_t, Δ_x and Δ_y are time step size, grid size in x direction and grid size in y direction, respectively. Shen et al. [34] proposed a first-order numerical scheme for spatial VO fractional advection-diffusion equation with a nonlinear source term and analyzed the stability and convergence of the scheme. Zhang et al. [35] constructed a novel implicit numerical method, which has first-order accuracy both in time and space for time fractional VO mobile–immobile advection–dispersion model.

All aforementioned numerical methods for VO FPDEs are of first-order accuracy with respect to time or space. In contrast, in the current work we derive two new approximation formulas of second-order accuracy for VO time fractional operator with order $0 < \alpha(t) < 1$ and $1 < \alpha(t) < 2$, respectively. Specifically, we adopt the following definition of VO [12]

$$ {}_0^C\mathcal{D}_t^{\alpha(t)} f(t) = \frac{1}{\Gamma(n-\alpha(t))} \int_0^t (t-s)^{n-\alpha(t)-1} f^{(n)}(s)\, ds, \quad n-1 < \alpha(t) < n. \tag{1.1} $$

Our objective is to apply these two new formulas to anomalous diffusion or dispersion and to exploit the advantages offered by the flexibility of VO, not only in modeling complicated and heterogeneous physics but also in accomplishing