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INITIAL VALUE PROBLEM FOR FRACTIONAL-ORDER DIFFERENTIAL EQUATIONS IN ANOMALOUS DIFFUSION PROCESSES

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Abstract: The study focuses on the initial value problem (IVP) for fractional-order differential equations in anomalous diffusion processes. Unlike classical diffusion, anomalous diffusion exhibits nonlocal temporal behavior and memory effects, which can be accurately described using fractional derivatives. The paper reviews analytical and numerical methods for solving IVPs, including Laplace and Fourier transforms, finite difference schemes, and physics-informed neural networks (PINNs). Applications of fractional IVPs in physics, biology, hydrology, and finance are highlighted, demonstrating their ability to model subdiffusive and superdiffusive transport. The integration of stochastic models, computational techniques, and experimental validation provides a comprehensive framework for understanding complex transport phenomena in heterogeneous media.

Keywords: anomalous diffusion, fractional-order differential equations, initial value problem, Caputo derivative, numerical methods, subdiffusion, superdiffusion, memory effects, fractional calculus, physics-informed neural networks.

ЗАДАЧА НАЧАЛЬНЫХ УСЛОВИЙ ДЛЯ ДИФФЕРЕНЦИАЛЬНЫХ УРАВНЕНИЙ ДРОБНОГО ПОРЯДКА В ПРОЦЕССАХ АНОМАЛЬНОЙ ДИФФУЗИИ

Аннотация: Данное исследование посвящено задаче начальных условий (ЗНУ) для дифференциальных уравнений дробного порядка в процессах аномальной диффузии. В отличие от классической диффузии, аномальная диффузия проявляет нелокальное временное поведение и эффекты памяти, которые можно точно описать с помощью дробных производных. Рассматриваются аналитические и численные методы решения ЗНУ, включая преобразования Лапласа и Фурье, схемы конечных разностей и нейронные сети с физическими ограничениями (PINN). Отмечены приложения дробных ЗНУ в физике, биологии, гидрологии и финансах, демонстрирующие их способность моделировать суб- и супердиффузионные процессы. Интеграция стохастических моделей, вычислительных методов и экспериментальной проверки обеспечивает комплексное понимание сложных транспортных явлений в неоднородных средах.

Ключевые слова: аномальная диффузия, дифференциальные уравнения дробного порядка, задача начальных условий, производная Капуто, численные методы, субдиффузия, супердиффузия, эффекты памяти, дробное исчисление, нейронные сети с физическими ограничениями.



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Anomalous diffusion represents a class of transport phenomena in complex media that cannot be adequately described by classical integer-order diffusion equations. Unlike normal diffusion, which follows Fick's laws and exhibits a linear mean squared displacement (MSD) over time, anomalous diffusion is characterized by nonlinear MSD, typically modeled as $\langle x^2(t) \rangle \sim t^\alpha$, where $\alpha \neq 1$. Subdiffusion ($\alpha < 1$) and superdiffusion ($\alpha > 1$) are the two primary types, reflecting hindrance and enhancement of particle motion, respectively. Such behaviors emerge in heterogeneous materials, porous media, crowded cellular environments, and turbulent flows, making anomalous diffusion a critical area of research in physics, biology, and engineering⁹.

Fractional calculus provides a natural framework to describe these processes, as it generalizes the concept of differentiation and integration to non-integer (fractional) orders. Fractional-order differential equations (FDEs) incorporate memory and hereditary properties of complex systems, which are essential to capture the long-range temporal correlations and spatial heterogeneity observed in anomalous diffusion. Among the commonly used fractional derivatives are the Caputo, Riemann-Liouville, and Grünwald-Letnikov definitions, each offering distinct mathematical and physical interpretations suitable for various applications¹⁰.

Formally, a fractional diffusion equation in one spatial dimension can be expressed as:

$$\frac{\partial^\alpha u(x,t)}{\partial t^\alpha} = D \frac{\partial^2 u(x,t)}{\partial x^2}, \quad 0 < \alpha \leq 1, \quad \frac{\partial^\alpha u(x,t)}{\partial x^2} = D \frac{\partial^2 u(x,t)}{\partial x^2}, \quad 0 < \alpha \leq 1,$$

where $u(x,t)$ is the particle concentration, D is the generalized diffusion coefficient, and $\frac{\partial^\alpha}{\partial t^\alpha}$ denotes the fractional derivative of order α with respect to time¹¹. The initial value problem (IVP) for such an equation involves determining $u(x,t)$ for $t > 0$ given initial conditions such as:

$$u(x,0) = f(x),$$

where $f(x)$ is a prescribed function representing the initial spatial distribution of particles. Unlike classical diffusion, the solution of fractional diffusion equations exhibits nonlocal temporal behavior, meaning the current state depends on the entire history of the process. This nonlocality introduces substantial challenges in both analytical and numerical treatment of the IVP.

Analytical approaches for solving IVPs in fractional diffusion often rely on Laplace and Fourier transform techniques. The Laplace transform with respect to time converts the fractional derivative into algebraic expressions, facilitating the solution in the transform domain. For example, applying the Laplace transform to the Caputo derivative yields:

⁹ Sokolov, I. M. (2012). Models of anomalous diffusion in crowded environments. *Soft Matter*, 8(35), 9043–9052.

¹⁰ Kilbas, A. A., Srivastava, H. M., & Trujillo, J. J. (2006). *Theory and Applications of Fractional Differential Equations*. Elsevier.

¹¹ Mainardi, F. (2010). *Fractional Calculus and Waves in Linear Viscoelasticity*. Imperial College Press.

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$$L\{\partial^\alpha u(x,t)\partial^\alpha t\} = s^\alpha \tilde{u}(x,s) - s^{\alpha-1} u(x,0), \quad L\left\{\frac{\partial^\alpha u(x,t)}{\partial t^\alpha}\right\} = s^\alpha \tilde{u}(x,s) - s^{\alpha-1} u(x,0),$$

where $\tilde{u}(x,s)$ is the Laplace transform of $u(x,t)$. The subsequent inversion of the Laplace transform allows recovery of the time-dependent solution, often expressed in terms of Mittag-Leffler functions, which generalize the exponential function and naturally describe the memory effects inherent in fractional-order dynamics¹².

Numerical methods are indispensable for IVPs of FDEs, particularly in higher dimensions or complex geometries where analytical solutions are not feasible. Finite difference schemes, finite element methods, and spectral methods have been adapted to fractional derivatives, ensuring stability and convergence while capturing the history-dependent behavior. The Grünwald-Letnikov approximation, for instance, discretizes the fractional derivative as a weighted sum over previous time steps, accurately representing the nonlocal memory effect¹³. Applications of fractional-order IVPs in anomalous diffusion span a wide spectrum. In biophysics, subdiffusive transport models explain the constrained motion of macromolecules in crowded intracellular environments. In hydrogeology, solute transport in heterogeneous aquifers exhibits non-Fickian behavior accurately captured by fractional diffusion models. In finance, the modeling of anomalous diffusion in asset prices informs risk assessment and derivative pricing.

The study of IVPs in fractional diffusion also intersects with stochastic processes. Continuous-time random walks (CTRWs) and Lévy flights provide microscopic interpretations of the fractional dynamics, linking probability distributions of waiting times and jump lengths to the fractional exponent α . This connection enhances the physical understanding of anomalous diffusion and guides the formulation of initial and boundary conditions in IVPs. The initial value problem for fractional-order differential equations in anomalous diffusion processes embodies the intricate interplay between nonlocal temporal behavior, complex media structures, and mathematical generalizations of classical derivatives. Advanced analytical and numerical techniques, coupled with experimental validation, are essential to accurately model and predict anomalous transport phenomena across disciplines. As computational capabilities expand and experimental methods improve, the study of fractional IVPs promises deeper insight into the fundamental mechanisms driving anomalous diffusion.

The investigation of initial value problems (IVPs) for fractional-order differential equations in anomalous diffusion continues to advance with the development of hybrid analytical-numerical techniques. In many practical scenarios, closed-form solutions are unavailable, particularly when the diffusion coefficient is space-dependent or when external forces and reaction terms are incorporated. In such cases, generalized numerical

¹² Gorenflo, R., & Mainardi, F. (1998). Fractional calculus: integral and differential equations of fractional order. *Fractals and Fractional Calculus in Continuum Mechanics*, 223–276.

¹³ Meerschaert, M. M., & Tadjeran, C. (2004). Finite difference approximations for fractional advection–dispersion flow equations. *Journal of Computational and Applied Mathematics*, 172(1), 65–77.



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schemes are implemented, often employing adaptive time-stepping to efficiently account for the nonlocal memory effects¹⁴. For example, the L1 scheme for Caputo derivatives has been widely adopted due to its first-order convergence and ease of implementation for uniform and nonuniform grids. The stability and convergence of numerical solutions for fractional IVPs require rigorous analysis. Unlike classical PDEs, fractional-order derivatives introduce long-term dependencies, which may amplify numerical errors if inappropriate discretization is used. The von Neumann stability analysis has been extended to fractional difference schemes, revealing that the memory kernel in the Grünwald-Letnikov approximation imposes additional constraints on the time step relative to the spatial discretization¹⁵. These constraints ensure that the fractional diffusion system evolves in a physically consistent manner, preserving non-negativity and mass conservation where applicable.

Another area of research involves the interplay between fractional IVPs and stochastic models. Fractional Fokker-Planck equations, derived from continuous-time random walks (CTRWs) with heavy-tailed waiting time distributions, are mathematically equivalent to fractional diffusion equations in the limit of long timescales. This equivalence enables the use of Monte Carlo simulations to approximate solutions of IVPs in highly complex geometries or with heterogeneous boundary conditions. Such simulations provide insight into the role of long-range correlations in anomalous transport, highlighting how initial distributions propagate differently compared to normal diffusion¹⁶.

In multidimensional systems, fractional diffusion equations take the form:

$$\frac{\partial^\alpha u(\mathbf{x}, t)}{\partial t^\alpha} = \nabla \cdot (D(\mathbf{x}) \nabla u(\mathbf{x}, t)) + R(u(\mathbf{x}, t), \mathbf{x}, t),$$

where $\mathbf{x} \in \mathbb{R}^n$, $D(\mathbf{x})$ is the spatially varying diffusion tensor, and R represents reactive or source terms. The IVP requires not only the specification of $u(\mathbf{x}, 0) = f(\mathbf{x})$, but also, in some formulations, fractional initial conditions for derivatives of order less than α . These conditions ensure the well-posedness of the problem and uniqueness of solutions under fractional calculus frameworks¹⁷. Experimental validation of fractional IVPs has gained prominence with high-resolution particle tracking and fluorescence correlation spectroscopy. In cellular biophysics, trajectories of macromolecules in crowded cytoplasm display subdiffusive behavior consistent with $\alpha \approx 0.7$, confirming the relevance of fractional models for IVPs in

¹⁴ Diethelm, K., Ford, N. J., Freed, A. D. (2002). A predictor-corrector approach for the numerical solution of fractional differential equations. *Nonlinear Dynamics*, 29(1–4), 3–22.

¹⁵ Sousa, E. (2012). Stability and convergence of finite difference schemes for fractional diffusion equations. *Applied Mathematical Modelling*, 36(12), 5663–5672.

¹⁶ Magdziarz, M., & Weron, A. (2007). Simulation of subdiffusion via Monte Carlo methods. *Physical Review E*, 75(5), 056702.

¹⁷ Kilbas, A. A., Srivastava, H. M., & Trujillo, J. J. (2006). *Theory and Applications of Fractional Differential Equations*. Elsevier.

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capturing realistic dynamics. Similarly, transport of contaminants in fractured rocks demonstrates non-Fickian dispersion, validating space-dependent fractional diffusion coefficients in multidimensional IVPs.

Recent advances in machine learning have also begun to influence the solution of fractional IVPs. Neural network-based solvers, particularly physics-informed neural networks (PINNs), have been employed to approximate solutions of fractional diffusion equations directly from initial and boundary data without explicit discretization¹⁸. These approaches are promising for large-scale problems where traditional numerical methods become computationally prohibitive. PINNs also offer the advantage of handling noisy experimental data, thereby bridging the gap between theoretical IVPs and real-world measurements.

Conclusion

The study of initial value problems (IVPs) for fractional-order differential equations in anomalous diffusion processes provides a powerful framework to model transport phenomena in complex media. Unlike classical diffusion, anomalous diffusion exhibits memory effects and nonlocal temporal behavior, which are naturally captured by fractional derivatives. Analytical methods, including Laplace and Fourier transforms, provide exact solutions in simple geometries, while numerical approaches, such as finite difference schemes and physics-informed neural networks, enable the solution of IVPs in more complex systems. Fractional IVPs find applications across physics, biology, hydrology, and finance, accurately describing subdiffusive and superdiffusive behaviors observed in experiments. Continued research integrating stochastic modeling, advanced computational methods, and experimental validation will deepen the understanding of anomalous transport and broaden the practical applications of fractional-order models.

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¹⁸ Pang, G., Lu, L., & Karniadakis, G. E. (2019). fPINNs: Fractional physics-informed neural networks. *SIAM Journal on Scientific Computing*, 41(4), A2603–A2626.



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