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Subdiffusive discrete time random walks via Monte Carlo and subordination

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ABSTRACT

A class of discrete time random walks has recently been introduced to provide a stochastic process based numerical scheme for solving fractional order partial differential equations, including the fractional subdiffusion equation. Here we develop a Monte Carlo method for simulating discrete time random walks with Sibuya power law waiting times, providing another approximate solution of the fractional subdiffusion equation. The computation time scales as a power law in the number of time steps with a fractional exponent simply related to the order of the fractional derivative. We also provide an explicit form of a subordinator for discrete time random walks with Sibuya power law waiting times. This subordinator transforms from an operational time, in the expected number of random walk steps, to the physical time, in the number of time steps.

1. Introduction

There has been a great deal of interest in recent years in solving partial differential equations (PDEs) with fractional order derivatives. This interest has been motivated by the recognition that physical properties, such as anomalous diffusion [1] and viscoelasticity [2], can be modelled using fractional order PDEs. A classic example is the time fractional subdiffusion equation,

$$\frac{\partial u}{\partial t} = D_\alpha \, {}_0\mathcal{D}_t^{1-\alpha} \frac{\partial^2 u}{\partial x^2}, \tag{1}$$

where ${}_0\mathcal{D}_t^{1-\alpha}$ denotes the Riemann–Liouville fractional derivative of order $1-\alpha$. This fractional PDE governs the evolution of the probability density for an ensemble of diffusing particles whose variance scales as a sublinear power law with time,

$$\mathbb{E}[\|x(t) - x(0)\|^2] \sim t^\alpha, \quad 0 < \alpha < 1. \tag{2}$$

Brownian motion, described by the standard diffusion equation, is recovered when $\alpha = 1$. The time fractional subdiffusion equation has been derived as a limit form of the evolution equation for the probability density describing an ensemble of continuous time random walks (CTRWs), characterized by power law waiting time densities and nearest neighbour, or Gaussian, step length densities [1]. The power law waiting time density models the phenomenon of trapping whereby the

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longer a particle remains at a site the more likely it is to continue waiting. The derivation, using CTRWs with power law waiting times, has also been extended to fractional Fokker–Plank equations [3–5] and fractional reaction–diffusion equations [6,7].

Algebraic approaches to solving fractional PDEs include the variational iteration method [8], the homotopy perturbation method [9], and the Admonian decomposition method [10]. Numerical approaches include explicit [11] and implicit [12] finite difference schemes, Galerkin methods [13], and spectral methods [14]. In earlier work, inspired by the CTRW method of deriving fractional PDEs, we introduced a numerical method for approximating solutions of fractional PDEs based on discrete time random walks (DTRWs) [15,16]. The DTRWs are characterized by a discrete waiting time probability mass function and a step-length probability mass function. With appropriately chosen, waiting time and step length, mass functions the generalized master equation for the evolution of the probability mass function, describing the position and location of an ensemble of DTRWs, limits to the same generalized master equation for the ensemble of CTRWs with power law waiting time densities. This correspondence can be exploited to provide an explicit finite difference scheme whose solution approximates the solution of the fractional PDE. This DTRW method can also be used to approximate solutions to fractional order ODE compartment models [17], and integer order advection–diffusion PDEs [18].

In this work we develop a Monte Carlo method for simulating DTRWs [15,16] that provides a numerical method for approximating the solution of the fractional subdiffusion equation. Monte Carlo methods based on simple discrete random walks have been widely employed in solving diffusion problems in a variety of application areas, from mathematical finance [19,20], to the simulation of chemical reactions [21], to mathematical biology [22].

In the DTRW that we introduced for anomalous subdiffusion [15,16] the waiting time between jumps is a simple renewal process [23], and the waiting time probability mass function is the Sibuya distribution [24,25] given by

$$\mathbb{P}[\text{Jump waiting time} = m] = \frac{\alpha}{m}\prod_{\ell=1}^{m-1}\left(1-\frac{\alpha}{\ell}\right).$$

The combination of this waiting time probability mass function together with nearest-neighbour jumps yields a process that is subdiffusive, in the diffusion limit of the space–time grid.

Monte Carlo path-wise simulations for calculating the ensemble average solution of the subdiffusive process out performs finite difference methods for small α, typically less than 3/4. The performance benefit is due to the semi-Markovian nature of the process. In the Monte Carlo simulations we do not need to know the history of a particle when choosing its next jump. Furthermore we find that the expected number of jumps for a trajectory up to a time point n scales as $\mathcal{O}(n^\alpha)$, meaning less jumps are required for small α. We find a closed form expression for the probability of a process undergoing k jumps up to time n,

$$\mathbb{P}[\text{Exactly } k \text{ jumps up to time } n] = (-1)^n \sum_{\ell=0}^{k}(-1)^\ell \binom{k}{\ell}\binom{(\ell+1)\alpha-1}{n}.$$

We use this expression to calculate expected computational complexity for a path-wise Monte Carlo simulation of our process, and compare it with the corresponding finite difference scheme that calculates the ensemble average result directly. The expression above furthermore enables us to find a closed form solution for the ensemble average, in a formula that is reminiscent of the subordination formula used to solve the subdiffusive time-fractional partial differential equation [26].

The remainder of this paper is as follows. In Section 2 we derive the generalized master equation for the ensemble average of discrete time random walk paths characterized by independently distributed waiting times and jump lengths. The particular cases of exponentially distributed and Sibuya distributed waiting times are discussed, leading to the standard diffusion equation, and the fractional diffusion equation, respectively. In Section 3 we describe the Monte Carlo method for approximating the solution of the fractional diffusion equation. In Section 4 we compute the computational complexity of calculating an ensemble of random paths. In Section 5 we derive the discrete subordination result linking the solution of the generalized master equation, with Sibuya distributed waiting times, to the solution of the generalized master equation with exponentially distributed waiting times. Finally, in Section 6 we present numerical results of the Monte Carlo path-wise simulations and make comparisons to known analytic solutions, as well as to numerical results based on the corresponding finite difference scheme. We show that CPU timing of the Monte Carlo simulations is consistent with the computational complexity analysis in Section 4.

2. Generalized master equations for an ensemble of discrete time random walks

We consider a random walker, which we refer to as a particle, to be traversing discrete space time. The particle undergoes a series of jumps from point to point. After each jump we draw a random waiting time, and after waiting at that point for that amount of time, the particle instantaneously jumps to some other point, chosen randomly from a jump probability distribution. Thus we generate a path by producing a series of independently distributed waiting times $W_k(\omega) \in \mathbb{N}$ and jumps $J_k(\omega) \in \mathbb{Z}$. The process can easily be generalised to d-dimensional space by allowing $J_k(\omega) \in \mathbb{Z}^d$, however for simplicity we only consider one spatial dimension here. The waiting time, and jumps, are both discrete renewal processes with