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Estimation of the smallest eigenvalue in fractional escape problems: Semi-analytics and fits

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ABSTRACT

Continuous time random walks with heavy tailed distributions of waiting times and jump lengths lead to situations when evolution of a probability density of finding a particle at given point at given time is described by the bi-fractional Smoluchowski–Fokker–Planck equation. A power-law distribution of waiting times results in very general properties of a survival probability which in turn can be used to estimate eigenvalues of some fractional operators. Here, the problem of numerical estimation of the smallest eigenvalues is discussed for the two generic problems: escape from a finite interval and the Kramers problem of escape from a potential well. We discuss both how to numerically obtain the (effective) smallest eigenvalue of the problem, and how it can be used in numerically assessing other important characteristics of the processes.

1. Introduction

Traditionally, it is assumed that diffusion is a memoryless process with Markovian increments leading to a Gaussian distribution of displacements. This is the natural consequence of the central limit theorem, stating that a sum of many independent bounded increments (or, generally, increments characterized by finite variance) converges in distribution to a Gaussian. Both assumptions underlying normal diffusion can be violated. Increments can follow a heavy tailed distribution, subsequent increments do not need to be independent, or the waiting time distribution between the steps or jumps can be characterized by the diverging mean. The most interesting situation takes place when both these assumptions are violated simultaneously.

There is a growing experimental evidence demonstrating occurrence of more general, heavy-tailed fluctuations. In particular, recorded examples include: diffusion in the energy space [1], exciton and charge transport in polymers under conformational motion [2], spectral analysis of paleoclimatic data [3,4], two-dimensional rotating flows [5]. In addition to examples showing more general jumps, there are also examples demonstrating slowing down of diffusion [6,7] due to anomalously long trapping events or other causes, see [8] for a short review of different models.

More general types of diffusion require special treatment and description which significantly departs from Markovian and/or Gaussian paradigm. Systems revealing anomalously long jumps or anomalously long trapping events no longer can be described by the standard diffusion equation. In context of anomalous diffusion fractional equations naturally emerge because long jumps lead to the fractional space derivatives while long rests result in the fractional time derivatives, see Section 2. The boundary-value problems for fractional diffusion equations are usually more complicated to solve than their standard diffusion analogs. The main difficulty is connected with formulating the correct boundary conditions for equations involving fractional space derivative. Spacial fractional derivatives originate due to long (non-local) jumps and discontinuous trajectories. The discontinuity of the trajectory leads to the necessity to take into account that, for example, an absorbing boundary at $x = x_0$, for the initial condition confined to $x < x_0$, implies that all particles attempting to cross it from left to right get absorbed "on the flight". This can be done either by considering non-local additional condition implying vanishing of the concentration for all $x \geqslant x_0$ [9], or by modifying the fractional space operator in such a way, that all particles attempting to cross the boundary essentially land on it [10,11]. Both variants make an already complex analytics of fractional equations even more complicated.

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Analytical solutions of fractional equations can be constructed in the simplest cases only [12–14], indicating strong necessity for development of numerical methods. These methods are of two general types: the first group focuses on the direct solving of fractional equations [15–23] while the second group approximates underlying stochastic process [24–26] whose probability density evolves according to the particular fractional equation. Solutions of the fractional equation are then reconstructed as histograms of this stochastic process. On the one hand, stochastic methods require generation of large number of realizations of stochastic processes. On the other hand, these methods are general, robust and relatively easy to implement because boundary conditions on a single trajectory level are straightforward. The accuracy of approximation is controlled both by the number of repetitions and time step of integration.

One of the typical methods of solving partial differential equation is separation of variables. This method can be extended to the fractional kinetic which can be described by a fractional diffusion equation. The applicability of factorization requires knowledge of eigenfunctions of spatial and temporal parts of the fractional operators. The knowledge of eigenfunctions (along with initial conditions) allows for construction of exact solutions of fractional equations. The construction of the spatial eigenfunctions however may pose considerable problems since usually there is only a limited or no knowledge about eigenfunctions and eigenvalues [27–30]. Moreover, presence of boundaries makes the complex problem even more sophisticated. On the other hand there are situations when the exact knowledge of all eigenfunctions is not necessary for obtaining the characteristics of interest, which might include the asymptotic behavior of probability densities and some other characteristics derived from the probability densities like: quantiles, survival probabilities, etc. In some situations the knowledge of temporal eigenfunctions and eigenvalues (determined by the spatial part of the operator) is sufficient to calculate system's characteristics. Semi-analytical methods provide a possibility to approximate eigenvalues which usually are not accessible analytically. More precisely, using (full) numerical solution it is possible to estimate the smallest (effective) eigenvalue by fitting procedure because asymptotic solution is dominated by the smallest eigenvalue. Next, using this estimate one can construct approximate solution based on the smallest (effective) eigenvalue. Finally, from an approximate solution required characteristics can be easily calculated. Here, semi-analytical methods are used to estimate smallest (effective) eigenvalues for two generic cases: escape from finite intervals and fractional Kramers problem. The estimated smallest (effective) eigenvalues are then used to approximate some characteristics of the escape process. The models considered are described in the next section. Results section presents the main outcome of numerical analysis. The paper is closed with summary and conclusions.

2. Models

We use semi-analytical methods in order to quantify some properties of systems which in the absence of boundaries would be described by the bi-fractional diffusion equation [31,32,25]:

$$\frac{\partial p(x,t)}{\partial t} = {}_0D_t^{1-\nu}\left[\frac{\partial}{\partial x}V'(x) + \sigma^\alpha \frac{\partial^\alpha}{\partial |x|^\alpha}\right] p(x,t). \tag{1}$$

The bi-fractional Smoluchowski–Fokker–Planck equation describes evolution of the probability density of finding a particle at time t in the vicinity of x. We restrict ourselves to the escape from finite intervals [33,34] and fractional Kramers problem [35,36].

In Eq. (1), ${}_0D_t^{1-\nu}$ denotes the Riemann–Liouville fractional derivative ${}_0D_t^{1-\nu} = \frac{\partial}{\partial t}{}_0D_t^{-\nu}$ defined by the relation

$${}_0D_t^{1-\nu} f(x,t) = \frac{1}{\Gamma(\nu)}\frac{\partial}{\partial t}\int_0^t dt' \frac{f(x,t')}{(t-t')^{1-\nu}} \tag{2}$$

and $\frac{\partial^\alpha}{\partial |x|^\alpha}$ stands for the Riesz–Weil fractional derivative with the Fourier transform

$$\mathcal{F}\left[\frac{\partial^\alpha}{\partial |x|^\alpha} f(x)\right] = -|k|^\alpha \hat{f}(x). \tag{3}$$

Within the complementary continuous time random walk framework, the fractional time derivative captures anomalously long waiting times ($p(t) \propto t^{-(\nu+1)}$ with $0 < \nu < 1$) while the fractional space derivative describes anomalously long jumps ($p(x) \propto |x|^{-(\alpha+1)}$ with $0 < \alpha < 2$). The same version of the fractional Smoluchowski–Fokker–Planck equation (1) corresponds to the situation when jumps are generated from α-stable densities [37–40] which in the symmetric case have the required $p(x) \propto |x|^{-(\alpha+1)}$ asymptotics. We refer to ν as the subdiffusion parameter and to α as the stability index. For $\alpha = 2$, the α-stable density is equivalent to the Gaussian distribution. In such a case, the fractional Riesz–Weil derivative is replaced by the standard second order derivative.

The fractional space derivative, see Eq. (3), originates due to non-local long jumps. Consequently, for $\alpha < 2$, the trajectories of the process whose evolution of the probability density is described by Eq. (1), are discontinuous. Discontinuity of trajectories requires special treatment because boundary conditions cannot be implemented in a typical point-wise manner. More precisely, the particle instead of hitting the boundary can jump over it. The two possibilities to resolve the difficulty were discussed above; here we use the first approach which can be easily implemented numerically on a single trajectory level, i.e. we use the subordination methods which are general and robust to exact values of parameters.

We are specially interested in the problem of first escape from the initial domain of motion which is restricted by absorbing boundaries. In particular, in the case of escape from finite intervals the motion of the particle is restricted to the $[-L, L]$ domain; the whole exterior of the $[-L, L]$ interval is absorbing. In addition to the escape from the finite intervals, we study the escape problem from the double well potential $V(x) = -ax^2/2 + bx^4/4$ (Kramers problem). Initially, we assume that the random walker is located in the middle of the interval (escape from finite intervals) or in the left potential well (fractional Kramers problem), see Fig. 1. For the escape from a finite interval, the process is restricted by boundaries located at $\pm L$. For the Kramers problem, states of the process are associated with minima of the double well potential, which are separated by the boundary located at the maximum of the potential.

The properties of first escape can be characterized by the first passage time density and the survival probability. From Eq. (1) the first passage time density can be obtained [41,42]

$$f(t) = f(t|x_0, 0) = -\frac{d}{dt}\int_\Omega p(x, t|x_0, 0)dx, \tag{4}$$

where Ω is domain of the motion and $p(x, t|x_0, 0)$ is the solution of Eq. (1) subject to the appropriate boundary and initial conditions [9,27]. The first passage time density is connected to the survival probability

$$S(t) = \int_\Omega p(x, t|x_0, 0)dx \tag{5}$$

by the relation

$$f(t) = -\frac{d}{dt}S(t). \tag{6}$$

The survival probability $S(t)$ is the probability that at time t a random walker is still in the $[-L, L]$ interval or on the left hand side the potential barrier, see Fig. 1. The survival probability $S(t)$ is related to the cumulative density of the first passage time $\mathcal{F}(t) = \int_0^t f(u)du = 1 - S(t)$.