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CAN ONE SEE A COMPETITION BETWEEN SUBDIFFUSION AND LÈVY FLIGHTS? A CASE OF GEOMETRIC-STABLE NOISE*

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Competition between subdiffusion and Lévy flights is conveniently described by the fractional Fokker–Planck equation with temporal and spatial fractional derivatives. The equivalent approach is based on the subordinated Langevin equation with stable noise. In this paper we examine the properties of such Langevin equation with the heavy-tailed noise belonging to the class of geometric stable distributions. In particular, we consider two physically relevant examples of geometric stable noises, namely Linnik and Mittag–Leffler. We describe in detail a numerical algorithm for visualization of subdiffusion coexisting with Lévy flights. Using Monte Carlo simulations we demonstrate the realizations as well as the probability density functions of the considered anomalous diffusion process.

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1. Introduction

In 1966 Mark Kac gave a famous lecture in the Leiden University with the dramatic title "Can one hear the shape of a drum?" The situation became even more dramatic, when a Physics Department secretary has replaced in the announcement "drum" by "dream" and the lecture room was

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full of psychiatrists from all over the Netherlands [1]. In his talk he asked if the shape of a planar region is determined by the spectrum of the Laplacian. The square roots of the eingenvalues of the Laplacian (frequencies) can be numerically computed if the shape is known. In his work [2] Kac proved that no other shape has the same spectrum as disc. In general, the answer is no, and was not solved by this paper, but almost 25 years later [3]. However, Kac's paper uses many interesting techniques to answer it partially. What is most important for our purposes, it uses the probabilistic techniques related to stochastic representation of solutions to elliptic partial differential equations. This paper is also famous as it was the basis of Kac's being awarded the Mathematical Association of America's (MAA) Chauvenet Prize. The Chauvenet Prize is awarded to the author of an outstanding expository article on a mathematical topic. Our days, since the spectrum contains geometrical information and since it is isometry invariant it is well suited to be used as a fingerprint (Shape-DNA) in computer graphics applications like database retrieval, quality assessment, and shape matching in fields like CAD, engineering or medicine, see [4].

Let us underline that a recognition of the close ties between Wiener's stochastic theory of Brownian motion and physics (Einstein–Smoluchowski approximate diffusion theory and not relativistic quantum mechanics) came about even earlier in Kac's two influential papers [5,6]. So, he can be considered as the father of stochastic representation methods in physics. In [5] he consequently introduced a discrete approach to the Einstein–Smoluchowski approximate theory. As Kac pointed out this approach was first suggested by Smoluchowski himself in connection with a free particle [7], when Kac developed it for other classical cases. It consists in treating Brownian motion as a discrete random walk. This is now achieved in physics by a very popular method of Continuous Time Random Walk (CTRW). The formal analogy between Feynman's path integrals (as presented in his Ph.D. Princeton 1942) and integrals appearing in Wiener's theory was striking for Kac and this led him in [6] to formalize the Feynman heuristic connection between the Schrödinger equation and the path integral into an "unassailable theorem". The theorem in question is often called the Feynman–Kac formula and there are literally dozens of proofs. The original proof of Kac was published in a brilliant paper [6]. For those who would like to learn more about Kac's rigorous approach and the above ties between mathematics and physics via stochastic representation we refer the readers to his two historical lecture notes [8, 9].

In the last years much attention has been devoted to the fractional Fokker–Planck equations (FFPEs) describing anomalous diffusion under the influence of an external field [10–13]. These equations provide a useful approach for the description of different types of dynamics in complex systems which are governed by anomalous diffusion [11] and nonexponential relaxation patterns [14]. Anomalous diffusion processes are characterized by the power law form $\langle(\Delta x)^2\rangle \propto Kt^\alpha$ of the mean-square displacement. According to the value of the anomalous diffusion index α, one distinguishes subdiffusion $(0 < \alpha < 1)$ and superdiffusion $(\alpha > 1)$, [11].

A different class of anomalous diffusion processes is formed by Lévy flights. They are characterized by the infinite second moment. Lévy flights are used to model variety of processes, such as bulk mediated surface diffusion with application to porous glasses and eye lenses, transport in micelle systems or heterogeneous rocks, special problems in reaction dynamics, in single molecule spectroscopy, quantum dots, protein dynamics, wait-and-switch relaxation and dielectric relaxation (see [11, 15–18] and references therein).

In this paper, using the method of stochastic representation via subordination [19,20], we propose a new model describing subdiffusion with Lévy flights. The Lévy flight type behavior is modeled by the Langevin equation driven by a heavy-tailed noise from the class of geometric stable distributions. The subdiffusive regime is obtained by the use of the inverse stable subordinator. We consider two physically relevant examples of geometric stable noises — Linnik and Mittag–Leffler. We describe in detail a numerical algorithm for visualization of subdiffusion coexisting with Lévy flights driven by such noises. Using Monte Carlo simulations we demonstrate the realizations as well as the probability density functions of the considered anomalous diffusion processes.

2. Competition between subdiffusion and Lévy flights

Competition (or coexistence) between subdiffusion and Lévy flights is conveniently described by the following fractional Fokker–Planck equation with temporal and spatial fractional derivatives [11]:

$$\frac{\partial w(x,t)}{\partial t} = {}_0D_t^{1-\alpha}\left[\frac{\partial}{\partial x}\frac{V'(x)}{\eta} + \nabla^\mu\right] w(x,t)\,. \tag{1}$$

Here, the operator

$${}_0D_t^{1-\alpha} f(t) = \frac{1}{\Gamma(\alpha)}\frac{d}{dt}\int_0^t (t-s)^{\alpha-1} f(s)ds\,, \tag{2}$$

$0 < \alpha < 1$, is the fractional derivative of the Riemann–Liouville type and ∇^μ, $0 < \mu \leq 2$, is the Riesz fractional derivative [21]. The occurrence of the operator ${}_0D_t^{1-\alpha}$ in Eq. (1) is induced by the heavy-tailed waiting times between successive jumps of the particle, whereas ∇^μ is related to the heavy-tailed distributions of the jumps in the underlying CTRW scenario. Eq. (1) was first derived in [22] from a generalized master equation. The constant η denotes the generalized friction constant. For $\mu = 2$, we obtain the FFPE describing subdiffusion in accordance with the mean-squared displacement [11, 23], while for $\alpha = 1$, Eq. (1) reduces to the Markovian Lévy flight [16]. The case $\mu = 2$, $\alpha = 1$ corresponds to the standard Fokker–Planck equation.

The equivalent approach to model competition between subdiffusion and Lévy flights is based on the subordinated Langevin equation with stable a noise [19, 20]. In the aforementioned references the authors have shown that the solution $w(x,t)$ of the FFPE (1) is equal to the probability density function (PDF) of the subordinated process

$$Y(t) = Z(S_t)\,. \tag{3}$$

This is the stochastic representation of the fractional Fokker–Planck dynamics (1). Here the parent process $Z(\tau)$ is defined as the solution of the stochastic differential equation (SDE)

$$dZ(\tau) = -V'(Z(\tau))\eta^{-1}d\tau + dL_\mu(\tau) \tag{4}$$

driven by symmetric μ-stable Lévy motion $L_\mu(\tau)$ with the Fourier transform $\langle e^{ikL_\mu(\tau)}\rangle = e^{-\tau|k|^\mu}$, [24]. The subordinator S_t, which is assumed to be independent of $L_\mu(\tau)$, is defined as

$$S_t = \inf\{\tau : U(\tau) > t\}\,. \tag{5}$$

Here, $U(\tau)$ denotes a strictly increasing α-stable Lévy motion [24], *i.e.* an α-stable process with Laplace transform

$$\left\langle e^{-kU(\tau)}\right\rangle = e^{-\tau k^\alpha}\,, \tag{6}$$

where $0 < \alpha < 1$. Many physical properties of *the inverse α-stable subordinator* S_t have been discussed in the papers [25–29]. The role of the subordinator S_t in the stochastic representation (3) is analogous to the role of the fractional Riemann–Liouville derivative (2) in the FFPE (1), since it introduces heavy-tailed rests of a test particle. Long jumps of the particle are induced by the stable noise $dL_\mu(\tau)$.

3. Geometric stable Lévy flights

Depending on the desired properties of the particle jumps, one can choose different noise distributions. We propose the following model $Y(t)$ describing coexistence between subdiffusion and Lévy flights, which is a generalization of (3)–(4):

$$Y(t) = X(S_t)\,. \tag{7}$$

Here, the parent process $X(\tau)$ is defined as the solution of the SDE

$$dX(\tau) = -V'(X(\tau))\eta^{-1}d\tau + dG_\mu(\tau)\,, \tag{8}$$

with $G_\mu(\tau)$ being the heavy-tailed μ-geometric stable Lévy process (see [30] and the next paragraph). The process S_t is the inverse α-stable subordinator. The introduced model describes the multiple trapping scenario, in which the trapping events are superimposed to the Lévy flight dynamics. In this scenario, the test particle moves according to the Lévy flight diffusion $X(\tau)$, however it gets successively immobilized in traps induced by the subordinator S_t.

Geometric stable laws [30] are the limiting distributions of the geometric compounding defined as

$$S_p = X_1 + X_2 + \ldots + X_{\nu_p}\,, \tag{9}$$

where ν_p is a geometric random variable with mean $1/p$ and probability function

$$P(\nu_p = k) = (1-p)^{k-1}p\,, \qquad k = 1, 2, 3, \ldots\,, \tag{10}$$

while X_i are i.i.d random variables independent of ν_p. The class of *geometric stable* laws is a four-parameter family denoted by $GS_\mu(\sigma, \beta, \lambda)$ with $0 < \mu \le 2$, $\sigma > 0$, $-1 \le \beta \le 1$, $\lambda \in \mathbb{R}$, and described by the characteristic function [30]

$$\psi(t) = [1 + \sigma^\mu |t|^\mu \omega_{\mu,\beta}(t) - i\lambda t]^{-1}\,, \tag{11}$$

where

$$\omega_{\mu,\beta}(x) = \begin{cases} 1 - \beta \mathrm{sign}(x)\tan(\pi\mu/2) & \text{if} \quad \mu \neq 1\,, \\ \\ 1 - \beta\frac{2}{\pi}\mathrm{sign}(x)\log|x| & \text{if} \quad \mu = 1\,. \end{cases} \tag{12}$$

A GS random variable Y has a representation in terms of independent standardized μ-stable and exponential variables S and W:

$$Y \overset{\mathrm{d}}{=} \begin{cases} \lambda W + W^{1/\mu}\sigma S, & \text{if} \quad \mu \neq 1\,, \\ \\ \lambda W + W\sigma S + \sigma W \beta (2/\pi)\log(W\sigma) & \text{if} \quad \mu = 1\,. \end{cases} \tag{13}$$

Geometric stable distributions share many features with the stable distribution as they are "heavy-tailed" and stable with respect to geometric summation. However, differently from the stable ones, their densities are more "peaked" and "blow-up" at zero, if $\mu < 1$. Densities of the stable and geometric stable distributions are presented in Fig. 1. The special cases of the geometric stable laws are [30]:

- Linnik distribution, with $\beta = 0$ and $\lambda = 0$,

- Mittag–Leffler distribution, with $\beta = 1$, $\lambda = 0$ and $0 < \mu < 1$.

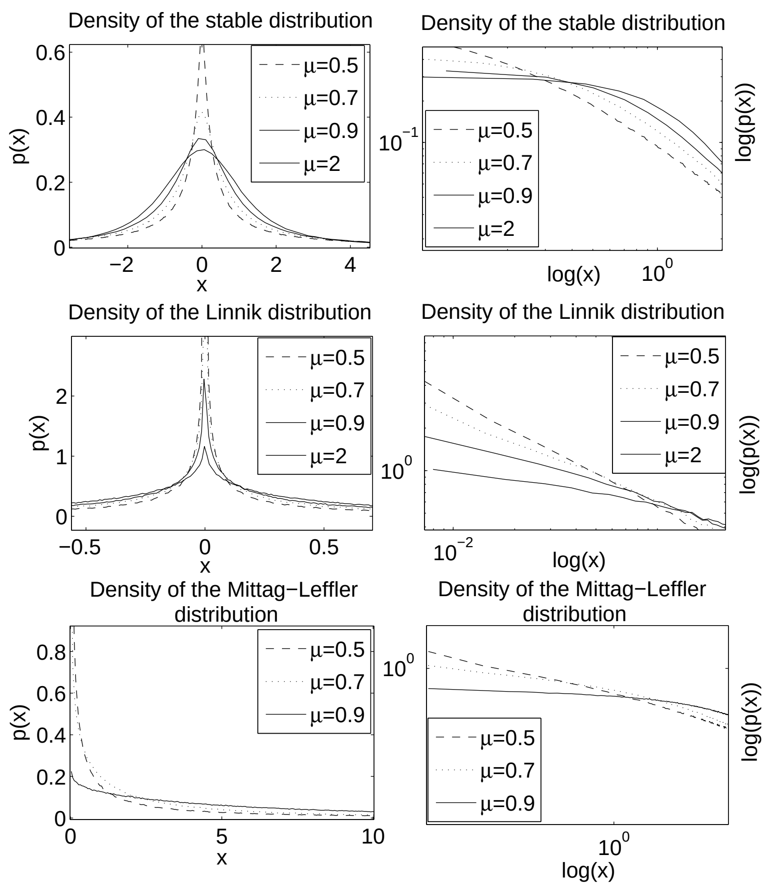

Fig. 1. Densities of the symmetric stable (top panel), Linnik (middle panel) and Mittag–Leffler (bottom panel) distributions in normal (left column) and log–log (right column) scale. The parameter σ is equal 1.

The Mittag–Leffler distribution is an important example of heavy-tailed waiting times that arises as the natural survival probability in relaxation theory [31–34] and in the CTRW approach to time-fractional Fokker–Planck equations [11,22,23,35–37]. Linnik is a symmetric counterpart of the Mittag–Leffler distribution.

As it is shown in Fig. 1, the Linnik density is symmetric with a characteristic peak at zero, while the Mittag–Leffler density is concentrated on the positive half-line. The tails of the stable as well as the geometric stable distribution are determined by the parameter μ as $P(Y > y) \sim Cy^{-\mu}$ (as $y \to \infty$) for $0 < \mu < 2$.

4. Simulation algorithm

In this section we show, how to simulate sample paths of the anomalous diffusion process with geometric stable noise (8). We concentrate on the Mitttag–Leffler and Linnik noises.

Recall that a stable random variable $S_\mu(\sigma, \beta, 0)$ can be generated as [38–40]

$$\begin{aligned} S_\mu(\sigma,\beta,0) \;=\; & c_1 \frac{\sin[\mu(V+c_2)]}{[\cos(V)]^{1/\mu}} \\ & \times \left(\frac{\cos[V-\mu(V+c_2)]}{W}\right)^{(1-\mu)/\mu}, \end{aligned} \tag{14}$$

where $c_1 = (1+\beta^2 \tan^2(\frac{\pi\mu}{2}))^{1/2\mu}$, $c_2 = \frac{\arctan(\beta \tan\frac{\pi\mu}{2})}{\mu}$, the random variable V is uniformly distributed on $(-\pi/2, \pi/2)$ and W has exponential distribution with mean 1. The random variable $S_\mu(\sigma, \beta, \lambda)$ is then given by

$$S_\mu(\sigma,\beta,\lambda) = S_\mu(\sigma,\beta,0) + \lambda\,. \tag{15}$$

To generate a geometric stable random variable Y we shall use representation (13). It gives a simple simulation algorithm:

1. Generate an exponential random variable
   $W = -\log(U)$, where U is uniformly distributed on $(0, 1)$.

2. Generate a stable random variable $S_\mu(1, \beta, \lambda)$, as described in (15).

3. For $\mu \neq 1$, put $Y = \lambda W + W^{1/\mu}\sigma S$.
   For $\mu = 1$, put $Y = \lambda W + W\sigma S + \sigma W\beta(2/\pi)\log(W\sigma)$.

Observe, that when generating the Linnik random variable $L_{\mu,\sigma}$ we get a mixture of the exponential and symmetric stable variables:

$$L_{\mu,\sigma} \stackrel{\mathrm{d}}{=} W^{1/\mu}\sigma S_\mu(1,0,0)\,, \tag{16}$$

while the Mittag–Leffler random variable $ML_{\mu,\sigma}$ is a mixture of exponential and totally skewed stable variables:

$$ML_{\mu,\sigma} \stackrel{\mathrm{d}}{=} W^{1/\mu}\sigma S_\mu(1,1,0)\,, \quad 0<\mu<1\,. \tag{17}$$

Suppose, we want to approximate the process $X(S_t)$ (7) on the lattice $\{t_i = i\Delta t : i=0,1,\ldots,N\}$, where $\Delta t = \frac{T}{N}$ and T is the time horizon. Recall that $X(\tau)$ is given by SDE (8) with Mittag–Leffler or Linnik noise, and S_t is the inverse α-stable subordinator. The proposed algorithm consists of two steps.

(I) Our first aim is to approximate the values $S_{t_0}, S_{t_1}, \ldots, S_{t_N}$ of the subordinator S_t. Therefore, we begin with approximating a realization of the strictly increasing α-stable Lévy motion $U(\tau)$ on the mesh $\tau_j = j\Delta\tau$, $j=0,1,\ldots,M$ (it is recommended to choose $\Delta\tau < \Delta t$). Using the standard method of summing increments of the process $U(\tau)$ we get

$$\begin{aligned} U(\tau_0) &= 0\,, \\ U(\tau_j) &= U(\tau_{j-1}) + \Delta\tau^{1/\alpha}\xi_j\,, \end{aligned} \tag{18}$$

where ξ_j are the i.i.d. totally skewed positive α-stable random variables. The procedure of generating realizations of ξ_j is the following [38–40]:

$$\xi_j = c_1 \frac{\sin[\alpha(V+c_2)]}{[\cos(V)]^{1/\alpha}} \left(\frac{\cos[V-\alpha(V+c_2)]}{W}\right)^{(1-\alpha)/\alpha}\,, \tag{19}$$

where $c_1 = [\cos(\pi\alpha/2)]^{-1/\alpha}$, $c_2 = \pi/2$, the random variable V is uniformly distributed on $(-\pi/2, \pi/2)$ and W has exponential distribution with mean 1. The iteration (18) ends, when $U(\tau)$ crosses the level T, *i.e.* when for some $j_0 = M$ we get $U(\tau_{M-1}) \le T < U(\tau_M)$. Since $U(\tau)$ is strictly increasing, such M always exists.

Now, for every element t_i of the lattice $\{t_i = i\Delta t : i=0,1,\ldots,N\}$, we find the element τ_j such that $U(\tau_{j-1}) < t_i \le U(\tau_j)$, and finally, from definition (5), we get that in such a case

$$S_{t_i} = \tau_j\,.$$

Since $U(\tau)$ is strictly increasing, the above method of finding the values S_{t_i}, $i=0,1,\ldots,N$, can be implemented efficiently [19].

(II) In the second step, we find the approximated values $X(S_{t_0})$, $X(S_{t_1})$, ..., $X(S_{t_N})$ of the subordinated process $X(S_t)$. Recall that from (I) we have at our disposal the approximations $S_{t_0}, S_{t_1}, \ldots, S_{t_N}$. First, we approximate the solution $X(\tau)$ of the SDE (8) on the lattice $\{\bar{\tau}_k = k\Delta\bar{\tau} : k = 0, 1, \ldots, L\}$, (it is recommended to choose $\Delta\bar{\tau} < \Delta t$). Here, the number L is equal to the first integer that exceeds the value $S_{t_N}/\Delta\bar{\tau}$. Employing the standard Euler scheme [24, 39] we obtain

$$\begin{aligned} X(\bar{\tau}_0) &= 0\,, \\ X(\bar{\tau}_k) &= X(\bar{\tau}_{k-1}) + \frac{V'(X(\bar{\tau}_{k-1}))}{\eta}\Delta\bar{\tau} + \bar{\xi}_k\,, \end{aligned} \tag{20}$$

for $k = 1, 2, \ldots, L$. Here $\bar{\xi}_k$ are i.i.d. random variables with the representation $\bar{\xi}_k \stackrel{\mathrm{d}}{=} \Gamma_{\Delta\bar{\tau}}^{1/\mu} S$, where Γ_t is the Gamma distributed random variable with parameter t and $S \stackrel{\mathrm{d}}{=} S_\mu(\sigma, \beta, 0)$ (compare with (13) for $\Gamma_1 = W$). The case $\beta = 1$, $0 < \mu < 1$ corresponds to the Mittag–Leffler case, whereas for $\beta = 0$, $0 < \mu < 2$ we get the Linnik noise. Finally, we obtain the approximate values $X(S_{t_0}), X(S_{t_1}), \ldots, X(S_{t_N})$ by finding for every t_i from the lattice $\{t_i = i\Delta t : i = 0, 1, \ldots, N\}$ such an index k that the condition $\bar{\tau}_k \leq S_{t_i} \leq \bar{\tau}_{k+1}$ holds true. Then, we get

$$X(S_{t_i}) = X(\bar{\tau}_k)\,, \tag{21}$$

$i = 0, 1, \ldots, N$. It is not recommended to use linear interpolation at this point, since the realizations of $X(\tau)$ are not continuous for $0 < \mu < 2$. By choosing the approximation of $X(S_{t_i})$ as in Eq. (21), we assure that the processes $X(\tau)$ and $X(S_t)$ have jumps of the same length.

5. Conclusions

Using the method of subordination and stochastic representation we analyze here subdiffusion with Levy flights. It is modeled by the subordinated Langevin equation driven by a heavy-tailed noise from the class of geometric stable distributions. We consider two physically relevant examples: the Linnik and Mittag–Leffler noise. The introduced algorithm allows us to simulate sample paths of the anomalous diffusion $X(S_t)$ for an arbitrary potential $V(x)$ and for the whole range of parameters $0 < \alpha < 1$ and $0 < \mu \leq 2$. Fig. 2 shows the sample paths of the subdiffusion process with Lévy flights driven by the stable and geometric stable distributions. The constant parts of the sample path indicate the heavy-tailed waiting times, while the long jumps of the particle confirm the heavy-tailed distributions of transfers in the underlying CTRW scheme. The subdiffusive behavior of the system is caused by the inverse α-stable subordinator, whereas the Lévy flight-type behavior is inherited from the parent process $X(\tau)$ described by the SDE (8). We believe that the stochastic methods presented here will contribute to a better understanding of physical systems displaying competition between subdiffusion and Lévy flights.

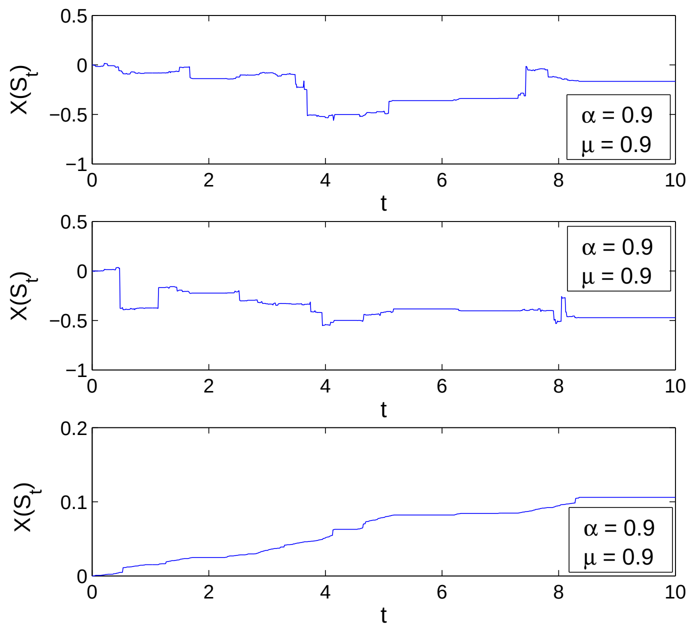

Fig. 2. Comparison of three sample realizations of the process $X(S_t)$ for different distributions of the jumps — stable (top panel), Linnik (middle panel) and Mittag–Leffler (bottom panel). The parameters are $\alpha = 0.9$, $\mu = 0.9$, $K = 1$, $\eta = 1$, $V(x) = \text{const}$.

This is a good occasion to clarify a pioneering role of Marian Smoluchowski [7] in developing the classical Fokker–Planck equation. For more details interested readers are referred to [8, 9, 41]. See also [42].

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