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Anomalous diffusion as modeled by a nonstationary extension of Brownian motion

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If the mean-square displacement of a stochastic process is proportional to t^{β}, $\beta \neq 1$, then it is said to be anomalous. We construct a family of Markovian stochastic processes with independent nonstationary increments and arbitrary but *a priori* specified mean-square displacement. We label the family as an extended Brownian motion and show that they satisfy a Langevin equation with time-dependent diffusion coefficient. If the time derivative of the variance of the process is homogeneous, then by computing the fractal dimension it can be shown that the complexity of the family is the same as that of the Brownian motion. For two particles initially separated by a distance x, the finite-size Lyapunov exponent (FSLE) measures the average rate of exponential separation to a distance ax. An analytical expression is developed for the FSLEs of the extended Brownian processes and numerical examples presented. The explicit construction of these processes illustrates that contrary to what has been stated in the literature, a power-law mean-square displacement is not necessarily related to a breakdown in the classical central limit theorem (CLT) caused by, for example, correlation (fractional Brownian motion or correlated continuous-time random-walk schemes) or infinite variance (Levy motion). The classical CLT, coupled with *nonstationary increments*, can and often does give rise to power-law moments such as the mean-square displacement.

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I. INTRODUCTION

Over the last decade, there has been a growing interest in non-Fickian or anomalous transport processes. The standard description of an anomalous process is one where the mean-square displacement goes asymptotically as time to some power, β, other than 1. If $0 \leq \beta < 1$, then the process is called subdiffusive and if $\beta > 1$, then it is superdiffusive. Lévy processes [1,2] that do not have a finite second moment, fall into the superdiffusive category. The case where $\beta = 1$ corresponds to a classical Brownian motion.

Subdiffusive and superdiffusive processes are the rule in many heterogeneous or preasymptotic systems. Subdiffusive processes appear in confined nanofilms [3–5], transport in natural porous media [6], fractal structures with holes over all length scales [7], charge-carrier transport in anomalous semiconductors [8,9], and NMR diffusometry on percolation structures [10]; see [11] for a review. Superdiffusion occurs in the atmosphere [12,13], in geologic formations [14–16], vortex arrays in rotating flows [17], and layered velocity fields [18], to name a few examples.

In one dimension a process $X(t)$ is said to be Brownian [19] if (a) every increment $X(t+s) - X(s)$ is normally distributed with mean zero and variance $\sigma^2 t$ where σ is fixed; (b) for every pair of disjoint time intervals (t_1, t_2) and (t_3, t_4), $t_1 < t_2 \leq t_3 < t_4$, the increments $X(t_4) - X(t_3)$ and $X(t_2) - X(t_1)$ are independent random variables with distribution given by (a); (c) $X(0) = 0$ and $X(t)$ is continuous at $t = 0$.

A standard Brownian motion has $\sigma = 1$; thus by the properties of a normal distribution, any Brownian motion, $X(t)$, can be made standard by replacing $X(t)$ with $X(t)/\sigma$. The Fokker-Planck equation for a Brownian process is the classical diffusion equation with constant diffusion coefficient.

The Lyapunov exponent is commonly used to quantify mixing in fluid mechanics and is defined as the exponential rate of separation, averaged over infinite time, of fluid parcels initially separated infinitesimally. That is, the Lyapunov exponent measures the average rate of exponential divergence of two infinitesimally close trajectories.

Unfortunately, the infinite time limit makes the Lyapunov exponent of limited practical value when dealing with experimental data. The spatial limiting process makes the Lyapunov exponent an even more difficult quantity to evaluate experimentally or numerically.

A generalization of the Lyapunov exponent, called the finite-size Lyapunov exponent (FSLE) [20–22], has been proposed to study the growth of noninfinitesimal perturbations (distance between trajectories) in dynamical systems. The FSLE, $\lambda_a(x)$, is defined by

$$\lambda_a(x) = [1/T_a(x)]\ln a \tag{1}$$

and is a measure of the growth rate of the mixing zone or alternatively a measure of the growth rate of the finite-size perturbations. Here T_a, the a time, is the average time it takes for two particles separated by a distance x initially to reach a separation of ax. Since ax is the threshold, a is called the threshold ratio. If x is thought of as a measure of the scale of

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the mixing layer in a dispersive flow, then $\lambda_a(x)$ measures the exponential rate of growth to scale ax,

$$\exp[\lambda_a(x)T_a(x)] = a. \quad (2)$$

By means of particle tracking algorithms, one can select nearby particles separated a given distance, say x, and then follow them by measuring the time $T_a(x)$ it takes for the separation to grow to ax. In the Brownian limit, it has been argued that the FSLE will be inversely proportional to the square of the initial separation and directly proportional to the classical diffusion coefficient [22]. In the case of symmetric α-stable Lévy particles, it has been argued [23,24] that $\lambda_a(x)$ is proportional to the diffusion coefficient and inversely proportional to x^α. The goals of this Brief Report are to show how by judiciously relaxing (a) above, we can create a spatially local, Markovian, stochastic process with any desired mean-square displacement and (b) to derive the FSLE for the process.

II. ONE-DIMENSIONAL COMPRESSED AND STRETCHED BROWNIAN MOTION

Let $H(t)$ be absolutely continuous with the non-negative derivative $h(t)$, i.e.,

$$H(t) = \int_0^t h(t')dt'. \quad (3)$$

We define a "compressed" ("stretched") Brownian process $X(t)$ as a process satisfying (b) and (c) above with (a) being replaced. (a′) Let $H(t) < t$ $[H(t) > t]$ be nonlinear and let $t > s$, then

$$X(t) - X(s) \sim N[0, H(t) - H(s)].$$

Clearly if $H(t)=t$ in (a′) then $X(t)$ is Brownian and except when $H(t)=t$, the process has nonstationary increments.

We next show that stretched and compressed Brownian motions satisfy the Ito stochastic ordinary differential equation (SODE),

$$dX = \sqrt{h(t)}d\eta(t), \quad (4)$$

where η is a standard Brownian motion. SODEs of this form have been studied extensively [25–28]. Assuming the particle is released at the origin, Eq. (4) is equivalent to

$$X(t) = \int_0^t \sqrt{h(s)}d\eta(s), \quad (5)$$

and hence

$$\langle X^2(t)\rangle = \left\langle \left[\int_0^t \sqrt{h(s)}d\eta(s) \right]^2 \right\rangle = \int_0^t h(s)ds = H(t), \quad (6)$$

where we have used the fact that $h(t)$ is deterministic and $\langle (d\eta)^2\rangle = dt$ [25]. From Eq. (5), $X(t)$ is a limit of a linear combination of Gaussians, and hence it is Gaussian and from Eq. (6) its variance is $H(t)$, so that $X(t) \sim N(0, H(t))$. Now $X(t) - X(s)$ and $X(s)$ are independent, so that $\mathrm{Var}\, X(t) = \mathrm{Var}[X(t)-X(s)+X(s)] = \mathrm{Var}[X(t)-X(s)] + \mathrm{Var}\, X(s)$ implies $\mathrm{Var}\, X(t) - \mathrm{Var}\, X(s) = \mathrm{Var}[X(t)-X(s)] = H(t) - H(s)$. Thus $X(t) - X(s) \sim N[0, H(t) - H(s)]$ which is (a′). The proofs of (b) and (c) are trivial.

Clearly, the Langevin (Fokker-Planck equation) for the transition density corresponding to Eq. (4) is a classical diffusion equation with time-dependent diffusion coefficient given by $h(t)/2$. A random-walk approximation for Eq. (4) takes the form

$$X(tn/M) - X(t(n-1)/M) \sim N(0, (t/M)h(tn/M)), \quad (7)$$

where t is a fixed time, t/M is a time increment, and n is the step.

III. MULTIDIMENSIONAL EXTENSIONS

There are several possible extensions; the simplest is to write the increments as

$$\mathbf{X}(t) - \mathbf{X}(s) \sim N(0, [H(t) - H(s)]\mathbf{Q}), \quad (8)$$

where each Q_{ij} is non-negative and independent of t and s. This simple extension allows one to study anisotropic processes with uniform scaling. A slightly more complicated extension takes the form

$$\mathbf{X}(t) - \mathbf{X}(s) \sim \prod_{i=1}^{3} N(0, H_i(t) - H_i(s)). \quad (9)$$

Here, in the principle directions, x_i, the component processes are independent and allowed to be compressed or stretched in different directions.

IV. EXAMPLES

A. Anomalous diffusion with power-law scaling

Here we set $h(t) = t^\alpha$, where $\alpha > -1$ [the integral of $h(t)$ diverges if $\alpha \leq -1$]. If $-1 < \alpha < 0$, then the process is compressed Brownian, if $\alpha = 0$ it is classical, and if $\alpha > 0$ it is stretched. We have $\langle |X(t)|^2 \rangle = t^{\alpha+1}/(\alpha+1)$. Thus the mean-square displacement is proportional to $t^{\alpha+1}$ so that the compressed case is subdiffusive and the stretched case is superdiffusive. Note that when $\alpha = 2$ we obtain Richardson superdiffusion [12] and when $\alpha = 1$, the system is ballistic. If a different power law is chosen in each direction then the Langevin equation takes the form

$$\partial f^\alpha / \partial t = -\boldsymbol{\nabla} \cdot \mathbf{q}^\alpha, \quad (10a)$$

$$\mathbf{q}^\alpha = -\mathbf{D}^\alpha(t) \cdot \boldsymbol{\nabla} f^\alpha, \quad (10b)$$

$$\mathbf{D}^\alpha(t) = \begin{pmatrix} q_1 t^{\alpha_1} & 0 & 0 \\ 0 & q_2 t^{\alpha_2} & 0 \\ 0 & 0 & q_3 t^{\alpha_3} \end{pmatrix}. \quad (10c)$$

B. Logarithmic subdiffusion

Here we take $h(t) = (t_0 + t)^{-1}$, where $t_0 > 0$. In this case, the mean-square displacement grows like $\ln(t_0 + t)$.

C. Multifractal diffusion

Here we take $h(t)=(t_0+t)^{\alpha(t)}$, where $\alpha(t)\geq -1$ and $t_0>0$. We call this multifractal diffusion in analogy to classical multifractal processes that have the same form of the mean-square displacement. In this case however, as pointed out next, the fractal dimension of the stochastic process does not change with $\alpha(t)$.

D. Complexity

Park *et al.* [29] computed the box fractal dimension of a stochastic process with nonstationary increments. Following his work [29], and provided that $h(t)$ is homogeneous [in the sense that $h(t)=t^\alpha$ implies $h(at)=a^\alpha h(t)$], we can show that the box dimensions of $\mathbf{X}^\alpha(t)$ is the same as the classical Brownian motion. Therefore the process $\mathbf{X}^\alpha(t)$ has the same complexity as the standard Brownian process. To date we have not succeeded in proving this result when $h(t)$ is not homogeneous.

V. FINITE-SIZE LYAPUNOV EXPONENT

The distribution of stretched/compressed Brownian motion is given by the solution of

$$\partial P/\partial t = Dh(t)\partial^2 P/\partial x^2, \tag{11}$$

where D is a constant. If we are computing the probability density of a particle, $D=\frac{1}{2}$, and if we are computing the probability density for the difference between two particle trajectories, $D=1$. This is because the diffusion coefficient is one-half times the derivative of the variance for these processes. Because the two particles have Gaussian distributions, the difference of two such particle trajectories is Gaussian with twice the variance as the motion of a single particle.

The reader should note [25] that Eq. (11) is the Eulerian counterpart to the Lagrangian SODE (4). However, Eq. (4) contains far more information than Eq. (11) does, as Eq. (4) describes specific particle trajectories rather than particle densities, i.e., many different SODEs can give rise to the same Langevin equation. For example, Dentz *et al.* [30] constructed a correlated random walk that does not satisfy the central limit theorem (CLT) but satisfies essentially the same Langevin equation as our process does.

For diffusion on the interval $[0,L]$ with absorbing boundaries, the boundary conditions are expressed mathematically as

$$P(0,t) = P(L,t) = 0, \tag{12}$$

with the initial condition

$$P(x,0) = \delta(x-x_0). \tag{13}$$

Note that the solution to this problem is given by

$$P(x,t) = \frac{2}{L}\sum_{n=1}^{\infty} \sin\left(\frac{\pi n x}{L}\right)\sin\left(\frac{\pi n x_0}{L}\right)e^{-[\pi^2 n^2 DH(t)/L^2]}. \tag{14}$$

Following Gitterman [31], we compute the mean first passage time (MFPT), T, for this process,

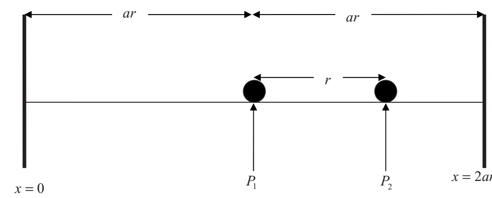

FIG. 1. Initial configuration of two particles (labeled as P_1 and P_2) and two passage planes at $x=0$ and $x=2ar$.

$$T = \int_0^L \int_0^\infty P(x,t)dtdx$$
$$= \sum_{n=1}^{\infty} \frac{2}{\pi n}[1-(-1)^n]\sin\left(\frac{\pi n x_0}{L}\right)\int_0^\infty e^{-[\pi^2 n^2 DH(t)/L^2]}dt. \tag{15}$$

We next compute $T_a^0(r)$, the time it takes for two particles separated by a distance r at $t=0$ to become separated by a distance ar for the first time. This can be accomplished by following the path laid out in [24]. We imagine two particles, separated by a distance r, each moving in the prescribed fashion. We attach the frame of reference to the first particle and fix passage planes at a distance ar from it (see Fig. 1).

In this frame of reference everything is fixed, except the second particle, which moves in this frame of reference with twice the variance. As noted above, this modifies the diffusion coefficient so that $D=1$ instead of $D=\frac{1}{2}$. The particles will be separated by a distance ar exactly when the second particle is at the passage planes. In this system, $T_a^0(r)$ is simply the MFPT with $L=2ar$ and $x_0=(a+1)r$. We obtain the following equation by inserting this information into the previous equation:

$$T_a^0(r) = \sum_{n=1}^{\infty} \frac{2}{\pi n}[1-(-1)^n]\sin\left(\frac{\pi n(a+1)}{2a}\right)$$
$$\times \int_0^\infty \exp\left(\frac{-\pi^2 n^2 H(t)}{(2ar)^2}\right)dt$$
$$= \sum_{k=1}^{\infty} \frac{4}{\pi(2k-1)}\sin\left(\frac{\pi(2k-1)(a+1)}{2a}\right)$$
$$\times \int_0^\infty \exp\left(\frac{-\pi^2(2k-1)^2 H(t)}{(2ar)^2}\right)dt. \tag{16}$$

Substituting this into the definition of the FSLE we obtain

$$\lambda_a^0(r) = \ln a \Bigg/ \sum_{k=1}^{\infty} \frac{4}{\pi(2k-1)}\sin\left(\frac{\pi(2k-1)(a+1)}{2a}\right)$$
$$\times \int_0^\infty \exp\left(\frac{-\pi^2(2k-1)^2 H(t)}{(2ar)^2}\right)dt. \tag{17}$$

Figure 2 provides a typical example of a family of FSLEs for $h(t)=t^\alpha$. It is important to note that the nonstationarity of the process requires the FSLE to be a function of time origin.

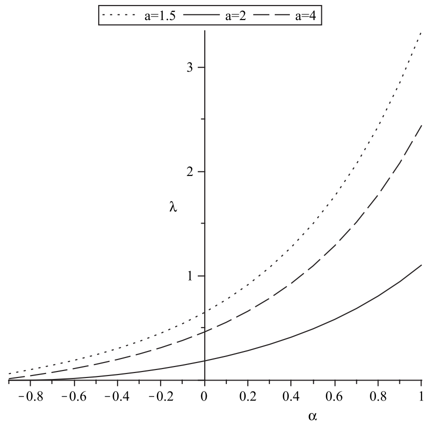

FIG. 2. Dependence of FSLE on α and a with $t_0=5$ and $r=1$.

VI. CONCLUSIONS

Our goal was to construct a family of Markovian stochastic processes that can be characterized by their first two moments with predefined mean-square displacement. To do so we relaxed the stationary-increment assumption associated with classical Brownian motion and showed, with our characterization, that the limit process has independent increments with $X(t)-X(s)\sim N(0,H(t)-H(s))$. This process can be generalized by assuming

$$\mathbf{X}^{\alpha}(t)-\mathbf{X}^{\alpha}(s)\sim\prod_{i=1}^{3}N(0,H_i(t)-H_i(s)). \tag{18}$$

Drift can be included for the constant velocity case by replacing the mean zero with $v_i(t-s)$ in the normal density of increments where v_i is the constant velocity in the x_i direction. Langevin equations for the transition density are classical diffusive with the time-dependent diffusion coefficient proportional to $h(t)$ or $D_i\sim h_i(t)$ in the multiple-dimension case.

A closed-form equation for the finite-size Lyapunov exponent was derived and a numerical example presented. If only the first two moments are required, or are all that is available, to characterize a physical process, then the model presented provides a simple and clear way of generating realizations and explaining experimental results.

One final point: it was stated in [11] on page 6 that a power-law mean-square displacement "is intimately connected with a breakdown of the central limit theorem, caused by either broad distributions or long-range correlations." The arguments put forward here illustrate that this does not have to be the case. In fact, we have relied solely on the classical central limit theorem for our analysis. It has been known for many years that upscaling (via projection operators, renormalization groups, generalized central limit theorems, matched asymptotics, etc.) may give rise to spatially nonlocal and non-Markovian processes, many of which have long-range correlations and power-law moments. What we have shown here is that classical CLT renormalization provides a spatially local and Markovian process which also may possess power-law moments. Thus while long-range correlations and breakdown of the CLT often lead to anomalous diffusion, they are not a necessary prerequisite.

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