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Characterizing anomalous diffusion by studying displacements

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ABSTRACT

Subordinated Lévy processes provide very diverse conceptual models for mass transport, beside other paradigms (e.g., fractional Brownian motion) generalizing Brownian motion. Some of that many models exhibit similar empirical Mean Squared Displacements growing non-linearly with time, while their increments have very different characteristic functions. In many media, such functionals can be directly measured, but accurate inversion methods adapted to them *and* to subordinated processes are still lacking. We show that each such process is associated to an operator that transforms the deviation from 1 of the characteristic function of its increments into a quantity that does not depend on the wave-number. We build an inversion method based on this property: it deduces the individual identity of each subordinated Lévy process from data sampling the characteristic functions of its increments.

1. Introduction

Transport experiments in complex media often show deviations from normal diffusion [1–3], manifested by empirical Mean Squared Displacement (MSD) $S(t)$ growing more slowly or more rapidly than time t (typically, $S(t) \propto t^a, a \neq 1$). However, many different stochastic models show such behavior, visible on [4] the empirical MSDs of subordinated stable processes, and on the true MSDs of fractional Brownian motion [5] or of other Gaussian models [6]. Yet, the increments of subordinated processes have characteristic functions that dramatically differ from Gaussian cases. Since describing increments is much easier in the Gaussian context (or for pure Lévy process), we concentrate our attention on Lévy processes subordinated by inverse Lévy subordinators.

Each of the latter is deduced from some Lévy process (which we call its parent) [7–9] by changing its time, independently of it: the clock time is replaced by the hitting time of a Lévy subordinator [10–14]. Subordinated processes describe a huge set of possibilities, and even the particular case of stable parent and strictly stable subordinator [4,15,16] describes a large subset that contains Brownian motion. In general, subordinated processes do not inherit the Markov property of their parent: their increments are neither independent, nor stationary. Nevertheless, describing their characteristic functions is facilitated if for parents and subordinators we write such functionals in exponential form, by means of Log-characteristic exponents. Provided we use these tools, the increments of general subordinated Lévy processes are not significantly more difficult to study than when we restrict our attention to the stable case.

Our interest in increments is enhanced by pulsed field gradient Nuclear Magnetic Resonance (NMR), an experimental method for characterizing mass transport [17]. This technique determines the distribution of the displacements Δx performed by spin bearers during a time interval of duration Δt: for a series of (small) Δt values, characteristic functions $\langle e^{ik\Delta x}\rangle$ are measured at several k values [17–19]. In fluids flowing through porous materials, for instance, pulsed field gradient

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NMR revealed [20] empirical MSDs growing super-linearly with time, a feature that many subordinated Lévy processes [4] share with many Gaussian processes [6]. Yet, [21] depicted displacement distributions by applying the (numerical) inverse Fourier transform to NMR data recorded in porous media: pictures displayed in this reference show non-Gaussian propagators resembling those of some subordinated processes. However, more quantitative tools are necessary to discriminate between models.

It turns out that a theorem of [22] describes the increments of the hitting times of general Lévy subordinators. It implies that each subordinated process is associated to a time-non local operator that characterizes its parent and its subordinator. This operator depends on the wave-number k, like the increment characteristic function. Yet, it transforms the deviation from 1 of the latter functional into a quantity that does not depend on k. This result holds in general, hence for stable parent subordinated by inverse strictly stable subordinator, whose one-time p.d.f solves a Doubly Fractional Fokker–Planck Equation (DFFPE), i.e. a partial differential equation involving derivatives of non-integer order w.r.t. time and space [23–27]. Other classes of parents and subordinators mentioned in the physical literature [10,14,28] are reminded in Appendix D. The aim of this paper is to demonstrate that the above mentioned operator gives us the opportunity of inverting pulsed field gradient NMR data.

To this end, we remind how each subordinated Lévy process is related to two pure Lévy processes, playing the roles of parent and subordinator. Then, we state a general expression for the characteristic function of the increments of each subordinated process: the deviation from 1 of this functional is transformed into a quantity independent of the wave-number, when we apply an operator (we call it specific) easily deduced from the Log-characteristic exponents of the parent and of the subordinator. Numerical experiments confirm the general formula. The principle of an inversion method adapted to data equivalent to the increment characteristic function is built upon the specific operator. We illustrate the method by applying it to numerical data, in the context of stable parent and strictly stable subordinator.

2. Lévy processes and subordinators

The characteristic function of each Lévy process is a powerful tool, which helps us describing the increments of each subordinated Lévy process.

2.1. General Lévy processes, and stable processes

From the definition of Lévy processes (here noted $\mathbb{L}_t$), we use that they are stochastically continuous, start from the origin (i.e. $\mathbb{L}_0 = 0$), and have stationary independent increments: for each $t_1 > 0$ and $\Delta t > 0$, $\mathbb{L}_{t_1+\Delta t} - \mathbb{L}_{t_1}$ is independent of the past, and equal in distribution to $\mathbb{L}_{\Delta t}$, a statement which we note $\mathbb{L}_{t_1+\Delta t} - \mathbb{L}_{t_1} =^d \mathbb{L}_{\Delta t}$ [8,9]. Hence, each Lévy process $\mathbb{L}_t$ is entirely described by its characteristic function $\langle e^{ik\mathbb{L}_t}\rangle$ [7], necessarily of the form of $e^{-t\Psi(k)}$, in which $\Psi(k)$ is the Log-characteristic exponent of $\mathbb{L}_t$. Strictly increasing Lévy processes are often used to represent irregular time schedules: they are called Lévy subordinators, and their Log-characteristic exponent Ψ is advantageously written in Laplace form, by setting $\Psi(is) = \psi(s)$, or equivalently $\langle e^{-s\mathbb{L}_t}\rangle = e^{-t\psi(s)}$. Laplace Log-characteristic exponents of Lévy subordinators are Bernstein functions [29]. For simplicity, throughout this paper k and s designate Fourier and Laplace variables.

Within Lévy processes, the stable [30,31] are characterized by the distribution of their time t value, a copy of that of a stable Lévy [32–34] random variable $L^{\alpha,\beta}$, whose characteristic function $e^{-\varphi_{\alpha,\beta}(k)}$ is recalled in Appendix A (the stability index α belongs to $]0,2]$, the skewness parameter β belongs to $[-1,1]$). We note $\mathcal{L}_t^{\alpha,\beta,D,v}$ the most general stable process, whose time t value is distributed as $vt + (Dt)^{1/\alpha}L^{\alpha,\beta}$: D is a scale factor. Such processes appear in different fields of science. When they are used to describe transport, the dimensionality of D is $\frac{[L]^\alpha}{[T]}$, that of v being $\frac{[L]}{[T]}$: v is a mean velocity if $L^{\alpha,\beta}$ has a finite average, i.e. for $\alpha > 1$. In this case, v is an important quantity, and measuring it motivates using pulsed field gradient NMR. The characteristic function of $\mathcal{L}_t^{\alpha,\beta,D,v}$ is $\langle e^{ik\mathcal{L}_t^{\alpha,\beta,D,v}}\rangle = e^{-Dt\varphi_{\alpha,\beta}(k)+ivkt}$, i.e. the Log-characteristic exponent $\Psi(k)$ is $-ikv + D\varphi_{\alpha,\beta}(k)$ in this case. Note that the one-time density of $\mathcal{L}_t^{\alpha,\beta,D,v}$ satisfies the space-fractional Fokker–Planck equation (FPE) [2,35] $\partial_t P(x,t) = \mathbb{A}_{\alpha,\beta,D,v}P(x,t)$, with

$$\mathbb{A}_{\alpha,\beta,D,v}P \equiv \partial_x[-vP] - \frac{D}{2\cos\left(\frac{\pi\alpha}{2}\right)}[(1+\beta)D^{\alpha}_{-\infty,x} + (1-\beta)D^{\alpha}_{x,+\infty}]P. \tag{1}$$

Left/right-sided Riemann–Liouville derivatives $D^{\alpha}_{-\infty,x}$ and $D^{\alpha}_{x,+\infty}$ [36,37] are briefly reminded in Appendix B. Stable processes include subordinators, in fact all the $\mathcal{L}_t^{\gamma,1,d,e}$ with positive d and e, the stability exponent γ ranging between 0 and 1. We pay special attention to the strictly stable case $e = 0$. Then, the variations of parameter d combine with that of D and v when we pass to subordinated processes, and among the strictly stable subordinators we only use (in this paper) the $T_z^\gamma = \mathcal{L}_z^{\gamma,1,\cos(\frac{\pi\gamma}{2}),0}$, of Laplace transform $\langle e^{-sT_z^\gamma}\rangle = e^{-zs^\gamma}$.

Pure stable processes describe diffusion in the stable case $\alpha = 2$, otherwise they account for extremely large displacements. Time-changing stable processes provides models for sub-diffusion [10,14] if $\alpha = 2$, and for super-diffusion or more complex behaviors if $\alpha < 2$ [4,15,16].