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Fractional diffusion: probability distributions and random walk models

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Abstract

We present a variety of models of random walk, discrete in space and time, suitable for simulating random variables whose probability density obeys a space–time fractional diffusion equation.

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1. Introduction

It is well known that the fundamental solution of the linear diffusion equation can be interpreted as a Gauss probability density function in space, evolving in time. The variance is proportional to the first power of time, a noteworthy property that can be understood by means of an unbiased random walk model for the Brownian motion.

In recent years evolution equations containing fractional derivatives have gained revived interest in that they are expected to provide suitable mathematical models

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for describing phenomena of anomalous diffusion in complex systems, see, e.g. [1–10]. For a recent review we refer the reader to Metzler and Klafter [11]. Anomalous diffusion can also be investigated in the framework of the Tsallis generalized statistical mechanics, see, e.g. [12]. Here we sketch our original approach to the topic that can offer some novel and inspiring inspections. In particular we pay attention to the fact that the fundamental solutions of the proposed fractional diffusion equations provide spatial probability densities evolving in time, related to *self-similar* stochastic processes, that we view as generalized (or *fractional*) diffusion processes to be properly understood through random walk models.

2. Probability distributions

By replacing in the standard diffusion equation

$$\frac{\partial}{\partial t} u(x,t) = \frac{\partial^2}{\partial x^2} u(x,t), \quad -\infty < x < +\infty, \quad t \geqslant 0\,, \tag{2.1}$$

where $u = u(x,t)$ is the (real) field variable, the second-order space derivative and the first-order time derivative by suitable *integro-differential* operators, which can be interpreted as a space and time derivative of fractional order, we obtain a generalized diffusion equation which may be referred to as the *space–time fractional* diffusion equation. We write this equation as

$${}_xD^{\alpha}_{\theta}\, u(x,t) = {}_tD^{\beta}_{*}\, u(x,t), \quad -\infty < x < +\infty, \quad t \geqslant 0\,, \tag{2.2}$$

where α, θ, β are the real parameters restricted as follows

$$0 < \alpha \leqslant 2, \quad |\theta| \leqslant \min\{\alpha, 2-\alpha\}, \quad 0 < \beta \leqslant 1\,. \tag{2.3}$$

In (2.2) ${}_xD^{\alpha}_{\theta}$ is the *Riesz–Feller* space-fractional derivative of order α and skewness θ, and ${}_tD^{\beta}_{*}$ is the Caputo time-fractional derivative of order β. The action of these fractional derivatives on sufficiently well-behaved functions are henceforth recalled.

For $0 < \alpha < 2$ the *Riesz–Feller* derivative of $f(x)$ reads, see, e.g. [13],

$$\begin{aligned} {}_xD^{\alpha}_{\theta}\, f(x) = \frac{\Gamma(1+\alpha)}{\pi} \Bigg\{ & \sin[(\alpha+\theta)\pi/2] \int_0^{\infty} \frac{f(x+\xi)-f(x)}{\xi^{1+\alpha}}\, \mathrm{d}\xi \\ & + \sin[(\alpha-\theta)\pi/2] \int_0^{\infty} \frac{f(x-\xi)-f(x)}{\xi^{1+\alpha}}\, \mathrm{d}\xi \Bigg\}\,. \end{aligned} \tag{2.4}$$

In terms of the Fourier transform we have

$$\mathscr{F}\{{}_xD^{\alpha}_{\theta}\, f(x);\kappa\} = -\psi^{\theta}_{\alpha}(\kappa)\hat{f}(\kappa), \quad \psi^{\theta}_{\alpha}(\kappa) = |\kappa|^{\alpha}\, \mathrm{e}^{\mathrm{i}(\operatorname{sign}\kappa)\theta\pi/2}\,, \tag{2.5}$$

where $\hat{f}(\kappa) = \mathscr{F}\{f(x);\kappa\} = \int_{-\infty}^{+\infty} \mathrm{e}^{+\mathrm{i}\kappa x} f(x)\,\mathrm{d}x$. In other words the symbol of the pseudo-differential operator ${}_xD^{\alpha}_{\theta}$ is required to be the logarithm of the characteristic function of the generic strictly stable probability density according to the Feller parameterization [14].

For $0 < \beta < 1$ the *Caputo* derivative of $f(t)$ reads, see, e.g. [15,16],

$${}_tD^{\beta}_{*}\, f(t) := \frac{1}{\Gamma(1-\beta)} \int_0^t \frac{f^{(1)}(\tau)\,\mathrm{d}\tau}{(t-\tau)^{\beta}}, \quad 0 < \beta < 1\,. \tag{2.6}$$

In terms of the Laplace transform we have

$$\mathscr{L}\{{}_tD_*^\beta f(t);s\} = s^\beta \tilde{f}(s) - s^{\beta-1} f(0^+), \quad 0<\beta<1\,, \tag{2.7}$$

where $\tilde{f}(s) = \mathscr{L}\{f(t);s\} = \int_0^\infty \mathrm{e}^{-st} f(t)\,\mathrm{d}t$. In other words the operator ${}_tD_*^\beta$ is required to generalize in the Laplace transform domain the first derivative keeping the standard initial value of the function.

The fundamental solution (or the *Green function*) of Eq. (2.2) is the solution corresponding to the initial condition $u(x,0^+) = \delta(x)$, that we denote by $G_{\alpha,\beta}^\theta(x,t)$. In the case of the standard diffusion equation (2.1) the Green function is nothing but the Gaussian probability density function with variance $\sigma^2 = 2t$, namely

$$G_{2,1}^0(x,t) = \frac{1}{2\sqrt{\pi}}\, t^{-1/2}\, \mathrm{e}^{-x^2/(4t)}\,. \tag{2.8}$$

In the general case we can prove that $G_{\alpha,\beta}^\theta(x,t)$ is still a probability density evolving in time with the noteworthy scaling property

$$G_{\alpha,\beta}^\theta(x,t) = t^{-\beta/\alpha} K_{\alpha,\beta}^\theta(x/t^{\beta/\alpha})\,. \tag{2.9}$$

Here $x/t^{\beta/\alpha}$ acts as the similarity variable and $K_{\alpha,\beta}^\theta(\cdot)$ as the *reduced Green function*. For the analytical and computational determination of the reduced Green function we can restrict our attention to $x>0$ because of the *symmetry relation* $K_{\alpha,\beta}^\theta(-x) = K_{\alpha,\beta}^{-\theta}(x)$. Mainardi et al. [17] have provided the Mellin–Barnes integral representation

$$K_{\alpha,\beta}^\theta(x) = \frac{1}{\alpha x}\,\frac{1}{2\pi\mathrm{i}} \int_{\gamma-\mathrm{i}\infty}^{\gamma+\mathrm{i}\infty} \frac{\Gamma(s/\alpha)\Gamma(1-s/\alpha)\Gamma(1-s)}{\Gamma(1-(\beta/\alpha)s)\Gamma(\rho s)\Gamma(1-\rho s)}\, x^s\,\mathrm{d}s, \quad \rho = \frac{\alpha-\theta}{2\alpha}\,, \tag{2.10}$$

where γ is a suitable real constant. We note that the Mellin–Barnes integral representation allows one to construct computationally the fundamental solutions of Eq. (2.1) for any triplet $\{\alpha,\beta,\theta\}$ by matching their convergent and asymptotic expansions [17]. Readers acquainted with Fox H functions can recognize in (2.10) the representation of a certain function of this class, see, e.g. [13,8]. Unfortunately, as far as we know, computing routines for this general class of special functions are not yet available.

We recall from [17] that for $\beta = 1$ and $0<\alpha<2$ (*space-fractional diffusion*) we recover the class $L_\alpha^\theta(x)$ of the strictly stable (non-Gaussian) densities exhibiting fat tails (with the algebraic decay $\propto |x|^{-(\alpha+1)}$) and infinite variance, whereas for $\alpha = 2$ and $0<\beta<1$ (*time-fractional diffusion*) the class of $\frac{1}{2}M_{\beta/2}(x)$ of the Wright type densities exhibiting stretched exponential tails and finite variance proportional to t^β. In the former case we obtain a special class of Markovian processes, called stable Lévy motions, which exhibit infinite variance associated to the possibility of arbitrarily large jumps (*Lévy flights*). In the latter case we obtain a class of stochastic processes which are non-Markovian and exhibit a variance consistent with slow anomalous diffusion. For the general *space–time-fractional* diffusion ($0<\alpha<2,\ 0<\beta<1$) we generate a class of densities (symmetric or non-symmetric according to $\theta=0$ or $\theta\neq 0$) which exhibit fat tails with an algebraic decay $\propto |x|^{-(\alpha+1)}$. Thus they belong to the domain of attraction of the Lévy stable densities of index α and can be referred to as *fractional stable densities*. The related stochastic processes possess the characteristics of the previous two classes. Indeed, they are non-Markovian (being $\beta < 1$) and exhibit infinite variance associated to the possibility of arbitrarily large jumps (being $\alpha < 2$).

3. Random walk models

To approximate the time evolution of our probability densities we have proposed finite difference schemes, discrete in space and time. By taking care in constructing these, they can be interpreted as random walk models for simulating particle paths by the Monte Carlo technique. By properly scaled transition to vanishing space and time steps, these models can be shown to converge to the corresponding continuous processes. For details we refer to the relevant papers of our group, see, e.g. [18–22]. Here our finite-difference schemes are adopted in some case-studies of Figs. 1–6 for producing *sample paths* and the corresponding *space-increments* of individual particles performing the random walks and for producing *histograms* of the approximate realization of the corresponding probability densities by simulating many

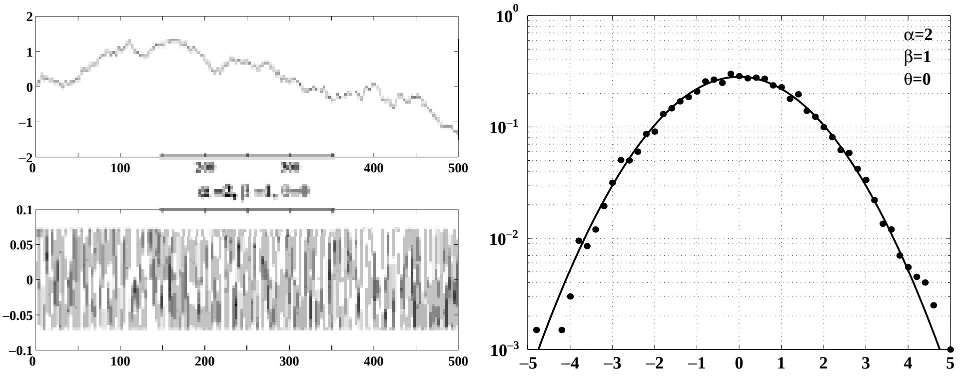

Fig. 1. Sample path with space increments (left) and histogram (right) for $\alpha = 2, \beta = 1, \theta = 0$.

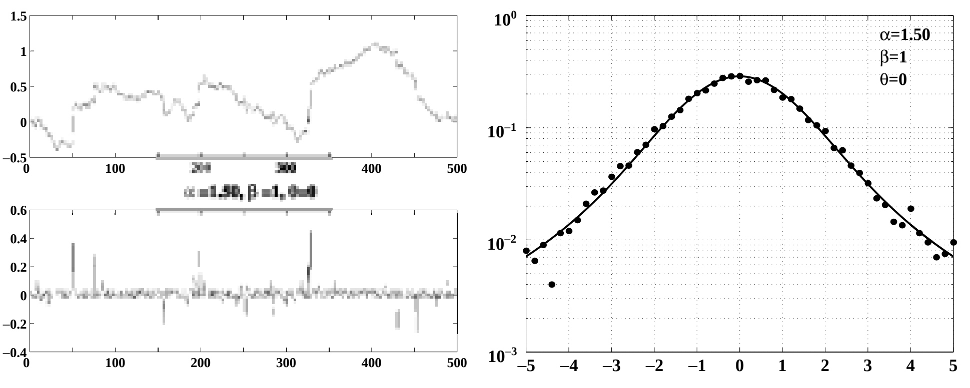

Fig. 2. Sample path with space increments (left) and histogram (right) for $\alpha = 1.50, \beta = 1, \theta = 0$.

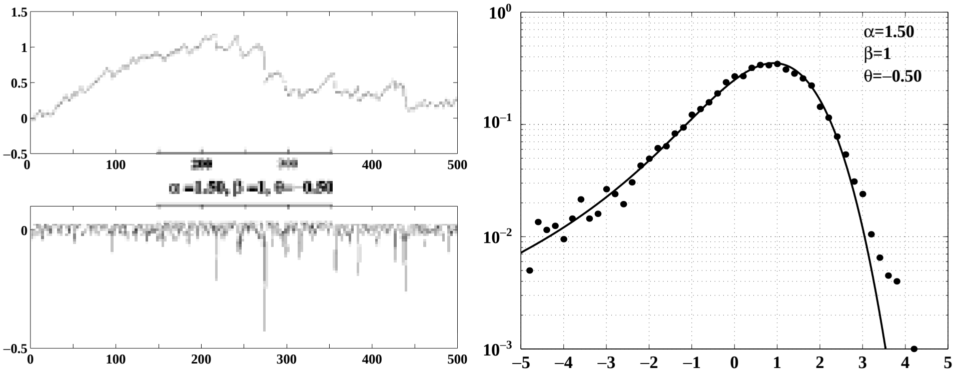

Fig. 3. Sample path with space increments (left) and histogram (right) for $\alpha = 1.50, \beta = 1, \theta = -0.50$.

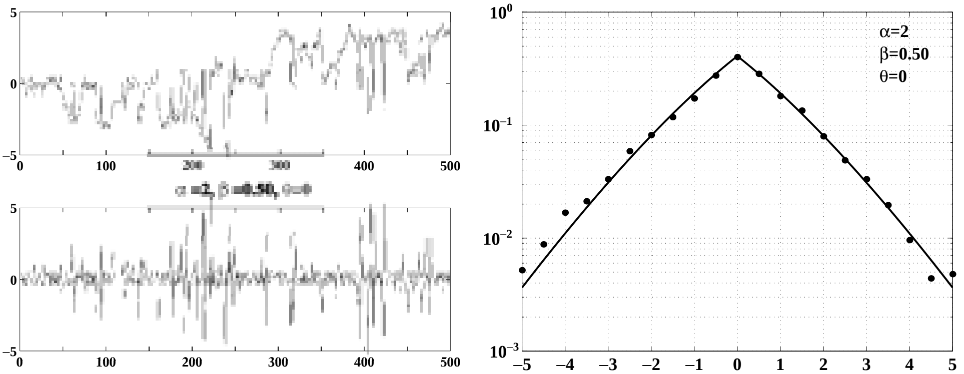

Fig. 4. Sample path with space increments (left) and histogram (right) for $\alpha = 2, \beta = 0.50, \theta = 0$.

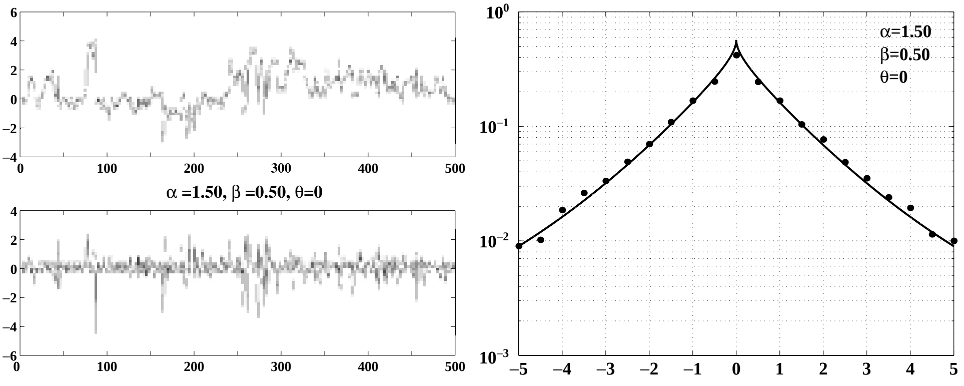

Fig. 5. Sample path with space increments (left) and histogram (right) for $\alpha = 1.50, \beta = 0.50, \theta = 0$.

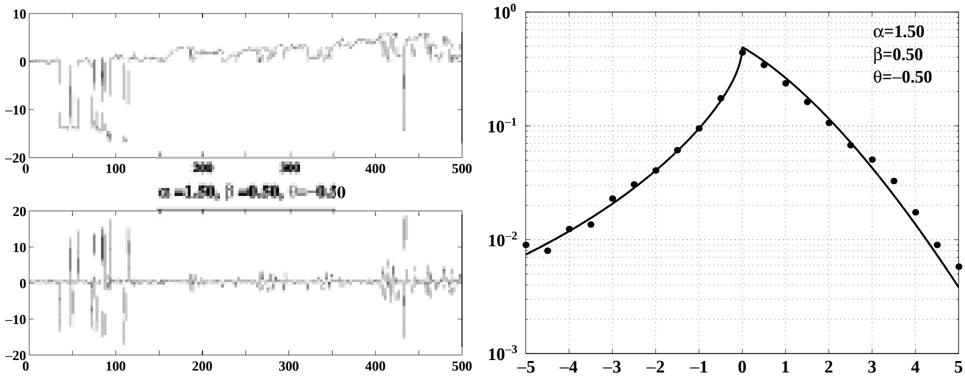

Fig. 6. Sample path with space increments (left) and histogram (right) for $\alpha = 1.50, \beta = 0.50, \theta = 0.50$.

individual paths with the same number of time steps and making statistics of the final positions of the particles. In the case $\beta = 1$ (no memory) our graphs nicely illustrate the contrast in the structure of trajectories for $\alpha = 2$ (continuity, tame behaviour) and $\alpha < 2$ (occurrence of large jumps). In the case $\beta < 1$ they exhibit the memory effect visible in a kind of stickiness combined with occasional jumps to points previously occupied.

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