

Multidimensional Advection and Fractional Dispersion*

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Extension of the fractional diffusion equation to two or three dimensions is not as simple as extension of the second-order equation. This is revealed by the solutions of the equations: unlike the Gaussian, the most general stable vector cannot be generated with an atomistic measure on the coordinate axes. A random combination of maximally skewed stable variables on the unit sphere generates a stable vector that is a general model of a diffusing particle. Subsets are symmetric stable vectors that have previously appeared in the literature, and the well-known multidimensional Brownian motion. A multidimensional fractional differential operator is defined in the process.

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1 Introduction

Diffusion equations that use fractional derivatives are attractive because they describe a wealth of continuous time random walks (CTRW [1]) that are good models of transport in real systems [2, 3, 4, 5]. Solutions to the fractional diffusion equations are Lévy motions, a generalization of Brownian motion using α -stable distributions [6]. Lévy motions are scaling limits of random walks with power-law transition probabilities, and their sample paths are random fractals [7] whose dimension α coincides with the order of the fractional derivative. Therefore, a strong motivation driving the specification of the fractional derivative operator is that the Green's function of the generalized diffusion equation is the full family of stable laws. A number of the derivations have been limited to special cases such as purely symmetric [8, 9] or maximally skewed [10, 11] particle transitions. More general derivations [4, 5, 12] recognize the need for weighted forward and backward fractional derivative operators in one-dimensional space.

We require an extension to higher dimensions, since problems of fractional diffusion are common in two and three dimensions. An asymmetric fractional derivative operator, which is a weighted average of directional derivatives in each radial direction, allows us to generate the full range of Lévy-stable motions. Since these processes can easily accommodate drift, we call these Fokker-Planck equations “fractional advection–dispersion equations”, noting that only the dispersion derivative is fractional, and that the fractional diffusion equation is a subset. We now use the term dispersion to include molecular diffusion and hydrodynamic dispersion [13]. We also concentrate only on spatially fractional dispersion, since extensions to fractional-in-time processes are straightforward [4, 5, 8, 9, 10].

2 Development

Let $X(t)$ be the position of a particle in d -dimensional Euclidean space \mathbb{R}^d at time $t \geq 0$. Let $P(x, t)$ denote the density of $X(t)$ where the vector $x = (x_1, \dots, x_d) \in \mathbb{R}^d$. The general advection–dispersion equation is

$$\frac{\partial P(x, t)}{\partial t} = -v \cdot \nabla P(x, t) + c \nabla_M^\alpha P(x, t) \quad (1)$$

where $v \in \mathbb{R}^d$ is the drift coefficient (velocity), $\nabla = (\partial/\partial x_1, \dots, \partial/\partial x_d)$, c describes the spreading rate of the dispersion, and ∇_M^α is the general (asymmetric) fractional derivative operator for $0 < \alpha \leq 2, \alpha \neq 1$. Using the Fourier transform convention $\hat{f}(k) = \int e^{-i\langle k, x \rangle} f(x) dx$ we specify this operator by requiring that $\nabla_M^\alpha f(x)$ has Fourier transform

$$\left[\int_{\|\theta\|=1} (i\langle k, \theta \rangle)^\alpha M(d\theta) \right] \hat{f}(k) \quad (2)$$

where $M(d\theta)$ is an arbitrary probability measure on the unit sphere $\{x \in \mathbb{R}^d : \|x\| = 1\}$. We call M the mixing measure, since (2) corresponds to a mixture of directional derivatives taken in each radial direction. Solutions to (1) with initial condition $P[X(0) = 0] = 1$ yield every possible multivariable Lévy motion $X(t)$ with index $0 < \alpha \leq 2, \alpha \neq 1$. The fractional diffusion process is made up of many infinitesimal particle jumps, and the mixing measure M gives the probability distribution for the radial direction of those jumps. When $\alpha = 2$ we get multivariable Brownian motion, and in this case (1) reduces to the classical advection–dispersion equation in \mathbb{R}^d . In one dimension we have $\|\theta\| = 1$ only for $\theta = \pm 1$ and so $\int (i\langle k, \theta \rangle)^\alpha M(d\theta) = p(ik)^\alpha + q(-ik)^\alpha$ where $p + q = 1$ and then (1) reduces to the general one dimensional fractional advection–dispersion equation [4, 5, 12].

Take Fourier transforms of (1) to obtain

$$\frac{d\hat{P}(k, t)}{dt} = -i\langle k, v \rangle \hat{P}(k, t) + c \left[\int_{\|\theta\|=1} (i\langle k, \theta \rangle)^\alpha M(d\theta) \right] \hat{P}(k, t) \quad (3)$$

so that for our initial condition $\hat{P}(k, 0) \equiv 1$ we obtain

$$\hat{P}(k, t) = \exp \left[-i\langle k, vt \rangle + ct \int_{\|\theta\|=1} (i\langle k, \theta \rangle)^\alpha M(d\theta) \right]. \quad (4)$$

Using $(iu)^\alpha = (e^{i\pi/2}u)^\alpha = |u|^\alpha \cos(\pi\alpha/2) \{1 + i\text{sign}(u) \tan(\pi\alpha/2)\}$ the right hand side above becomes

$$\exp \left[-i\langle k, vt \rangle + ct \int_{\|\theta\|=1} |\langle k, \theta \rangle|^\alpha \cos\left(\frac{\pi\alpha}{2}\right) \{1 + i\text{sign}(\langle k, \theta \rangle) \tan\left(\frac{\pi\alpha}{2}\right)\} M(d\theta) \right] \quad (5)$$

which is the Fourier transform of an arbitrary multivariable stable distribution with index $\alpha \neq 1$, compare [6] p.65. Thus the Green's function solution to (1) yields the entire class of multivariable Lévy motions for $\alpha \neq 1$.

The asymmetric fractional derivative operator ∇_M^α in (1) is a mixture of fractional directional derivatives. The directional derivative $D_\theta f(x) = \langle \theta, \nabla f(x) \rangle = \sum_j \theta_j \partial f(x) / \partial x_j = dg/ds$ at $s = 0$ where $g(s) = f(x + s\theta)$. Its Fourier transform is $\sum_j \theta_j i k_j \hat{f}(k) = i\langle k, \theta \rangle \hat{f}(k)$ since $i k_j \hat{f}(k)$ is the Fourier transform of $\partial f(x) / \partial x_j$. We can define fractional derivatives using convolutions of generalized functions in real space, or products in Fourier space [14]. The scalar fractional derivative is

$$D_+^\alpha g(s) = \frac{1}{\Gamma(n - \alpha)} \frac{d^n}{ds^n} \int_0^\infty r^{n-\alpha-1} g(s-r) dr$$

where $n = 1 + [\alpha]$ is the smallest integer greater than α , and it is easy to check that this convolution integral has Fourier transform $(iu)^\alpha \hat{g}(u)$ [5, 14]. Take the derivative inside the

integral and integrate by parts to obtain

$$D_+^\alpha g(s) = \frac{1}{\Gamma(-\alpha)} \int_0^\infty r^{-\alpha-1} g(s-r) dr$$

a convolution of generalized functions [14] p.154. The fractional order directional derivative $D_\theta^\alpha f(x)$ is defined by $D_+^\alpha g(s)$ evaluated at $s = 0$, where $g(s) = f(x + s\theta)$. Taking a mixture over the unit sphere $\|\theta\| = 1$ we get the convolution formula

$$\nabla_M^\alpha f(x) = \frac{1}{\Gamma(-\alpha)} \int_{\|\theta\|=1} \int_0^\infty r^{-\alpha-1} f(x-r\theta) dr M(d\theta) \quad (6)$$

whose Fourier transform is given by (2). If $M(d\theta) = m(\theta)d\theta$ and the constant c_d is the volume of the unit sphere in \mathbb{R}^d then a change of variables yields

$$\begin{aligned} \nabla_M^\alpha f(x) &= \frac{1}{\Gamma(-\alpha)} \int_{\|\theta\|=1} \int_0^\infty r^{-\alpha-1} f(x-r\theta) dr m(\theta) d\theta \\ &= \frac{1}{dc_d \Gamma(-\alpha)} \int_{\|\theta\|=1} \int_0^\infty r^{-\alpha-d} m(\theta) f(x-r\theta) dc_d r^{d-1} dr d\theta \\ &= \frac{1}{dc_d \Gamma(-\alpha)} \int_{y \in \mathbb{R}^d} \|y\|^{-\alpha-d} m\left(\frac{y}{\|y\|}\right) f(x-y) dy \end{aligned}$$

a ‘‘hypersingular integral with homogeneous characteristic’’ [14] p.518. When $m(\theta)$ is a constant function this integral reduces to the well-known convolution equation for the Riesz fractional derivative $\nabla^\alpha f(x)$ [14] p.483. We can also write (6) in the compact form $\nabla_M^\alpha f(x) = \int_{y \neq 0} f(x-y) \phi(dy)$ where $\phi(dy) = r^{-\alpha-1} dr M(d\theta) / \Gamma(-\alpha)$ in polar coordinates.

When $\alpha = 2$ the mixing measure M determines the covariance matrix. In this case the integral in equation (2) reduces to

$$- \int_{\|\theta\|=1} \left(\sum_{j=1}^d k_j \theta_j \right)^2 M(d\theta) = (ik) A (ik)^T \quad (7)$$

where the matrix $A = (a_{ij})$ with $a_{ij} = \int \theta_i \theta_j M(d\theta)$. Then (1) reduces to the classical advection–dispersion equation with $\nabla_M^\alpha = \nabla A \nabla^T = \sum_{i,j} a_{ij} \partial^2 / \partial x_i \partial x_j$ and

$$\hat{P}(k, t) = \exp[-i\langle k, vt \rangle - ct k A k^T]$$

which is the Fourier transform of a Gaussian with mean vt and covariance matrix $2ctA$, so we recover multivariate Brownian motion with drift. When $M(d\theta) = M(-d\theta)$ the integral in equation (2) reduces to

$$\frac{1}{2} \int_{\|\theta\|=1} (i\langle k, \theta \rangle)^\alpha + (i\langle k, -\theta \rangle)^\alpha M(d\theta) = \cos\left(\frac{\pi\alpha}{2}\right) \int_{\|\theta\|=1} |\langle k, \theta \rangle|^\alpha M(d\theta) \quad (8)$$

using $(iu)^\alpha + (-iu)^\alpha = 2|u|^\alpha \cos(\pi\alpha/2)$. Furthermore, if $M(d\theta)$ is uniform then $X(t)$ is symmetric stable and by (4) its density $P(x, t)$ has Fourier transform

$$\hat{P}(k, t) = \exp\left[-i\langle k, vt \rangle + ca_d t \|k\|^\alpha \cos\left(\frac{\pi\alpha}{2}\right)\right]$$

where the constant $a_d = \int |\theta_1|^\alpha M(d\theta)$ depends only on α and the dimension d of the space.

3 Discussion

Every stable random vector is of the form $b + UR$ where U is a random unit vector and R is a stable random variable which is maximally skewed and independent of U . The solution $X(t)$ to (1) is of this form with mean $b = vt$ and $P[U \in A] = M(A)$. Since $X(t)$ is a Markov process with stationary independent increments, the probability distribution M governs the direction of infinitesimal jumps. Numerical simulation of the fractional dispersion process $X(t)$ can be accomplished by adding small jumps $X(t + \Delta t) - X(t)$ of stable random vectors. Each jump is of the form $v\Delta t + UR$ where the jump direction U has probability

distribution M on the unit sphere. In terms of the standard parameterization for stable random variables [6], the jump size R is centered α stable with skewness $+1$ and scale σ satisfying $\sigma^\alpha = -c\Delta t \cos(\pi\alpha/2)$, so R can be simulated using the formula of Kanter [15]. For $\alpha < 2$ the fractional dispersion $X(t)$ is symmetric if and only if jumps in any direction are equally likely, while $X(t) = (x_1(t), \dots, x_d(t))$ has independent components $x_j(t)$ if and only if jumps are restricted to the coordinate axes [6] p.68. For $\alpha = 2$ both randomly directed and orthogonal jumps generate the same Brownian motion. This property is unique to the multivariate normal [16] p.258. Different mixing measures M yield different processes when $\alpha < 2$, while for $\alpha = 2$ we saw in (7) that the moments of M suffice to parameterize the dispersion process.

Lévy motions are scaling limits of random walks. Suppose $Z, Z_1, Z_2, Z_3, \dots, Z_n$ are independent and identically distributed random vectors in \mathbb{R}^d . If the rescaled random walk $a(\lambda)(Z_1 + \dots + Z_{[\lambda t]}) \Rightarrow L(t)$ as $\lambda \rightarrow \infty$ then $L(t)$ is a Lévy motion [17]. If $E\|Z\|^2 < \infty$ then $a(\lambda) = \lambda^{-1/2}$ and $L(t)$ is a Brownian motion. If we have $P[\|Z\| > r] \sim Cr^{-\alpha}$ and $P[\|Z\| > r, Z/\|Z\| \in A] \sim P[\|Z\| > r]M(A)$ as $r \rightarrow \infty$, then we get convergence with $a(\lambda) = \lambda^{-1/\alpha}$ and $L(t)$ is a Lévy process with index $\alpha < 2$ and mixing measure M [17]. Hence the fractional dispersion process $X(t) = vt + L(t)$ described by (1) gives a very robust model for particle motions. Only some generic tail properties of the jumps must be specified, and every possible limiting process is obtained.

The formula (5) for the Fourier transform of $X(t)$ is computed using the Lévy measure $\phi_t(dy) = ct \alpha r^{-\alpha-1} dr M(d\theta) / \Gamma(-\alpha)$, see [6] p.66. When $\alpha < 2$ the general convergence criterion for rescaled random walks is $\lambda P[a(\lambda)Z \in A] \rightarrow \phi_1(A)$ as $\lambda \rightarrow \infty$ [18]. The same Lévy measure ϕ_1 appears in the formula for the generator of the convolution semigroup

$\{P(x, t) : t \geq 0\}$ [19]. Point process theory says that $X(t)$ is the limit of compound Poisson random vectors, where $\phi_t(dy)$ gives the intensity of jumps of size y [20]. Finally, convolution with a Lévy measure is the simplest way to describe the full range of fractional derivatives. In our development, we obtained the formula $c\nabla_M^\alpha f(x) = \int_{y \neq 0} f(x - y)\phi_1(dy)$. This surprising connection between Lévy measures and fractional derivatives (or Riesz potentials) is new even in \mathbb{R}^1 .

4 Summary

The connection between certain stochastic processes and their governing partial differential equation is well known. In particular, Brownian motion implies a second-order diffusion equation [19]. We have shown a similar implication between the superset of diffusive motions – the stable Lévy motions – and the fractional advection–dispersion equation. The implication is shown by the n-dimensional fractional derivative defined as a convolution with a Lévy measure. The motions described by the fractional equation derived herein are characterized by occasional large jumps [6, 21]. The particle paths are fractals whose dimension corresponds to the order of the fractional derivative [7]. The motions can be symmetric or have any degree of skewness in several dimensions. One should expect skewed and fractional molecular diffusion in the midst of high chemical gradients and concentrations [4]. Dissolved solutes moving through porous aquifer material may exhibit nearly symmetric [22] to highly skewed [23] dispersion.

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