

Chapter 11

Fractional Calculus, Anomalous Diffusion, and Probability

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Ideas from probability can be very useful to understand and motivate fractional calculus models for anomalous diffusion. Fractional derivatives in space are related to long particle jumps. Fractional time derivatives code particle sticking and trapping. This probabilistic point of view also leads to some interesting extensions, including vector fractional derivatives, and tempered fractional derivatives. This paper reviews the basic ideas along with some practical applications.

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1. Introduction

The connection between the deterministic diffusion equation, and probabilistic Brownian motion, is a powerful and useful idea that has been exploited in many forms. The basic idea is that $p(x, t)$, the probability density function (PDF) of a Brownian motion stochastic process $B(t)$, solves the partial differential equation $\partial_t p = \partial_x^2 p$. On one hand, this means that solutions to a deterministic partial differential equation provide valuable information about random evolution. On the other hand, simulations of a random process can be used to generate numerical solutions to a deterministic model, a method called particle tracking. More fundamental is that the random path of a particle, described by the Brownian motion process,

provides a physical explanation for diffusion. Even in a completely deterministic derivation of the diffusion equation, in terms of flux and conservation of mass, random particle motions are the basic driving force.

Anomalous diffusion occurs when a cloud of particles spreads in a different manner than the traditional diffusion equation predicts. Fractional diffusion equations have become popular as the most reasonable and tractable models for anomalous diffusion. The traditional diffusion equation governs a Brownian motion, the long-time limit of a simple random walk with independent and identically distributed (IID) particle jumps (X_n). The approximation is a result of the central limit theorem of probability, and assumes finite first and second moments for the particle jumps.

If the jumps have power law probability tails, $\mathbb{P}(|X_n| > r) \approx r^{-\alpha}$ with $0 < \alpha < 2$, then the moment conditions are violated, and the random walk behavior is anomalous. In this case, the random walk limit is a stable Lévy motion $A(t)$ with index α , a natural mathematical extension of Brownian motion [45]. The PDF of the stable limit solves a space-fractional diffusion equation $\partial_t p = \partial_x^\alpha p$ that reduces to the traditional form when $\alpha = 2$. The underlying probability model gives a specific physical meaning for the fractional derivative in space: It codes large particle jumps, that lead to anomalous super-diffusion.

Note that the power law index α in the probability of long jumps equals the order of the fractional space derivative. A third interpretation for the index α comes from considerations of fractals and self-similarity. The path of a Brownian particle in space traces out a random fractal of dimension two, while a Lévy stable particle draws a fractal of dimension α , see [51]. This is closely connected to the idea of a self-similar stochastic process, the relation $B(ct) \approx c^{1/2}B(t)$ or $A(ct) \approx c^{1/\alpha}A(t)$ between processes rescaled in space and time. The self-similarity index $H = 1/\alpha$, also called the Hurst index, provides a useful way to categorize diffusion models. In traditional diffusion, with $H = 1/2$, a plume of diffusing particles spreads away from their center of mass at the rate t^H , which is evident from the scaling. The case $H > 1/2$ is called super-diffusion since particles spread at a faster rate.

Anomalous sub-diffusion is a model for particle sticking or trapping. Suppose that each particle jump X_n occurs at the end of a random waiting time J_n , with $\mathbb{P}(J_n > t) \approx t^{-\beta}$ for some $0 < \beta < 1$. This is called a continuous time random walk (CTRW), but it is really just a simple random walk in spacetime. The CTRW has a long-time limit density that solves a time-fractional diffusion equation $\partial_t^\beta p = \partial_x^2 p$ that reduces to the traditional form when $\beta = 1$. This shows that the time-fractional derivative models time delays between particle motion. Again, the order of the fractional derivative

is the same number that controls the probability model. The limit process is a time-changed Brownian motion $B(E_t)$ where the fractal time $E_{ct} \approx c^\beta E_t$, which leads to $B(E_{ct}) \approx c^{\beta/2} B(E_t)$. Since the Hurst index $H = \beta/2 < 1/2$, a plume of particles spreads slower than traditional diffusion. When long waiting times are combined with long particle jumps, a spacetime fractional diffusion equation $\partial_t^\beta p = \partial_x^\alpha p$ governs the CTRW limit, a process with $A(E_{ct}) \approx c^{\beta/\alpha} A(E_t)$. This can be sub-diffusive, super-diffusive, or even represent an anomalous diffusion that spreads with the same rate $H = 1/2$ as a Brownian motion.

The remainder of this chapter reviews some of the mathematics behind the fractional diffusion equation and its underlying stochastic process. We will also introduce some useful extensions and variations, including fractional vector calculus for vector-valued diffusions, and tempered models that smoothly interpolate between traditional and fractional diffusions. A more complete and detailed development of the ideas presented here can be found in the forthcoming book [36].

2. Fractional Derivatives and Probability

In this section, we introduce fractional derivatives from two different points of view: Differential equations, and probability. Then we will show that both points of view are really just two aspects of the same idea. Recall that the first derivative $\partial_x f(x) = \lim_{h \rightarrow 0} h^{-1} \Delta f(x)$ where the difference

$$\Delta f(x) = f(x) - f(x - h).$$

For positive integers α , $\partial_x^\alpha f(x) = \lim_{h \rightarrow 0} h^{-\alpha} \Delta^\alpha f(x)$, where

$$\begin{aligned} \Delta^2 f(x) &= (f(x) - f(x - h)) - (f(x - h) - f(x - 2h)) \\ &= f(x) - 2f(x - h) + f(x - 2h), \\ \Delta^3 f(x) &= f(x) - 3f(x - h) + 3f(x - 2h) - f(x - 3h) \\ &\vdots \\ \Delta^\alpha f(x) &= \sum_{m=0}^{\alpha} (-1)^m \binom{\alpha}{m} f(x - mh), \end{aligned}$$

where the Binomial coefficients

$$g_m = \binom{\alpha}{m} = \frac{\alpha!}{m!(\alpha - m)!} = \frac{\Gamma(\alpha + 1)}{\Gamma(m + 1)\Gamma(\alpha - m + 1)}.$$

For $\alpha > 0$, the fractional derivative $\partial_x^\alpha f(x) = \lim_{h \rightarrow 0} h^{-\alpha} \Delta^\alpha f(x)$ where

$$\Delta^\alpha f(x) = \sum_{m=0}^{\infty} \binom{\alpha}{m} (-1)^m f(x - mh). \tag{1}$$

This is actually the same formula as before, since $g_m = 0$ for $m > \alpha$ when α is an integer. Note that the integer derivative is a local operator, since it only depends on values of f near x , while the nonlocal fractional derivative depends on values of f in $(-\infty, x]$. Numerical analysis of fractional differential equations is based on (1).

The traditional diffusion equation is the result of two basic ideas: The concentration of particles $p(x, t)$, at location x and time t , must obey conservation of mass $\partial_t p = -\partial_x q$, where the particle flux $q(x, t)$ follows Fick's Law $q = -\mathcal{D} \partial_x p$. Fick's Law $q \Delta x \approx -\mathcal{D} \Delta p$ formalizes the empirical observation that particles cross a boundary between regions of differing concentration at a rate proportional to the difference in concentrations. The combination of these two laws gives the diffusion equation $\partial_t p = \mathcal{D} \partial_x^2 p$, where now we explicitly show the diffusivity \mathcal{D} . Implicit in Fick's law is the idea that all particles move at more or less the same velocity, so that we can account for flux over an interval of length $h = \Delta x$ in terms of the local difference in concentration $\Delta p = p(x, t) - p(x - h, t)$.

In fractional diffusion, a fractional Fick's law $q \Delta x \approx -\mathcal{D} \Delta^{\alpha-1} p$ for $1 < \alpha < 2$ recognizes the possibility that, when particle velocities are sufficiently heterogeneous, the flux can also depend on concentrations far upstream. The relative contributions of those concentrations depend on the weights in (1). Using Stirling's formula $\Gamma(x + 1) \sim \sqrt{2\pi x} x^x e^{-x}$ as $x \rightarrow \infty$ you can check that

$$w_m = (-1)^m \binom{\alpha}{m} \sim \frac{-\alpha}{\Gamma(1-\alpha)} m^{-1-\alpha} \text{ as } m \rightarrow \infty. \tag{2}$$

In fact, $w_0 = 1$, $w_1 = -\alpha$, $w_2 = \alpha(\alpha - 1)$ and so forth. The binomial formula states that

$$(1 + z)^\alpha = \sum_{m=0}^{\infty} \binom{\alpha}{m} z^m \tag{3}$$

for any complex $|z| \leq 1$ and any $\alpha > 0$. Set $z = -1$ to check that the weights w_m in (1) sum to zero, which ensures that all the mass leaving any given location arrives at some point downstream. The proportion of

particles transported m steps downstream falls off like a power law. Now the space-fractional diffusion equation

$$\partial_t p(x, t) = \mathcal{D} \partial_x^\alpha p(x, t) \tag{4}$$

comes from combining the fractional Fick's law and conservation of mass. The Fourier transform (FT)

$$\hat{f}(k) = \int_{-\infty}^{\infty} e^{-ikx} f(x) dx$$

converts differential equations to algebra, since $\partial_x^\alpha f(x)$ has FT $(ik)^\alpha \hat{f}(k)$. When α is a real number, this provides another equivalent definition of the fractional derivative (or fractional integral, if $\alpha < 0$). By the binomial formula (3) and the fact that $f(x - h)$ has FT $e^{-ikh} \hat{f}(k)$, $\Delta^\alpha f(x)$ has FT

$$\sum_{m=0}^{\infty} \binom{\alpha}{m} (-1)^m e^{-ikmh} \hat{f}(k) = (1 - e^{-ikh})^\alpha \hat{f}(k)$$

and then the FT of $h^{-\alpha} \Delta^\alpha f(x)$ is

$$h^{-\alpha} (ikh)^\alpha \left(\frac{1 - e^{-ikh}}{ikh} \right)^\alpha \hat{f}(k) \rightarrow (ik)^\alpha \hat{f}(k) \quad \text{as } h \rightarrow 0$$

by a Taylor series expansion $e^z = 1 + z + z^2/2! + \dots$. Take FT in the fractional diffusion equation (4) to get

$$\partial_t \hat{p}(k, t) = \mathcal{D} (ik)^\alpha \hat{p}(k, t)$$

and solve to get $\hat{p}(k, t) = \exp(t\mathcal{D}(ik)^\alpha)$. Inverting the FT in the case $\alpha = 2$ gives a normal density

$$p(x, t) = \frac{1}{\sqrt{4\pi\mathcal{D}t}} \exp\left(-\frac{x^2}{4\mathcal{D}t}\right) \tag{5}$$

which is the point source solution of the traditional diffusion equation. In the case $0 < \alpha < 2$, the solution is a Lévy stable PDF with index α . Usually, this PDF cannot be written in closed form.

Next we consider the fractional diffusion equation from the point of view of probability. The random particle jump X_n has PDF $f(x)$ with FT

$$\hat{f}(k) = \int_{-\infty}^{\infty} \left(1 - ikx + \frac{1}{2!}(ikx)^2 + \dots \right) f(x)dx = 1 - ik\mu_1 - \frac{1}{2}k^2\mu_2 + \dots,$$

where the p th moment

$$\mu_p = \int_{-\infty}^{\infty} x^p f(x)dx. \tag{6}$$

The random walk $S(n) = X_1 + \dots + X_n$ gives the particle location after n IID jumps. If we take centered jumps with $\mu_1 = 0$ and finite variance $\mu_2 = 2D$, then $\hat{f}(k) = 1 - Dk^2 + \dots$, the PDF of $S([nt])$ has FT $\hat{f}(k)^{[nt]}$, and the rescaled sum $S([nt])/\sqrt{n}$ has FT

$$\hat{f}(k/\sqrt{n})^{[nt]} = \left(1 - \frac{Dk^2}{n} + \dots \right)^{[nt]} \rightarrow e^{-tDk^2} \quad \text{as } n \rightarrow \infty.$$

Inverting the FT shows that the rescaled random walk converges in the limit to a Brownian motion $B(t)$ with PDF (5), the same formula that solves the traditional diffusion equation. This is the traditional central limit theorem (CLT) of probability. Figure 1 illustrates the random walk convergence, as the number of jumps increases, to a Brownian motion path, a continuous (but not differentiable) random fractal of dimension $3/2$.

For particle jumps with heavy tails $\mathbb{P}(X > x) \sim Dx^{-\alpha}/\Gamma(1 - \alpha)$, the jump PDF

$$f(x) \sim D \frac{\alpha}{\Gamma(1 - \alpha)} x^{-\alpha-1} \tag{7}$$

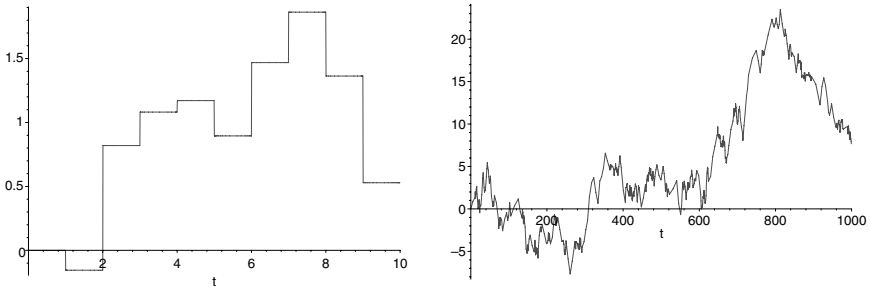


Fig. 1. Random walk simulation, showing convergence to Brownian motion.

and some moments μ_p are undefined, because the integral (6) does not converge, so the traditional CLT is not valid. If $1 < \alpha < 2$ and $\mu_1 = 0$, then a Tauberian theorem [18] shows that X has FT

$$\hat{f}(k) = 1 + \mathcal{D}(ik)^\alpha + \dots$$

and the rescaled random walk $n^{-1/\alpha}S([nt])$ has FT

$$\hat{f}(k/n^{1/\alpha})^{[nt]} = \left(1 + \frac{\mathcal{D}(ik)^\alpha}{n} + \dots\right)^{[nt]} \longrightarrow e^{t\mathcal{D}(ik)^\alpha} \quad \text{as } n \rightarrow \infty. \quad (8)$$

Inverting the FT shows that the rescaled random walk with heavy tail jumps converges in the limit to an α -stable Lévy motion $A(t)$, whose PDF solves the fractional diffusion equation (4). This is the Kolmogorov–Feller CLT [18]. Figure 2 illustrates the random walk convergence to the stable limit with fractal dimension $2 - 1/\alpha$. Note that the large jumps persist in the limit.

Check using (5) or its FT that Brownian motion scales according to $B(ct) \approx c^{1/2}B(t)$. The well-known PDF is bell-shaped, symmetric, with rapidly decreasing tails, and spreads like $t^{1/2}$ due to this scaling. The FT $\hat{p}(k, t) = \exp(t\mathcal{D}(ik)^\alpha)$ of the Lévy motion makes it evident that $A(ct) \approx c^{1/\alpha}A(t)$. Figure 3 shows the evolution of the stable PDF in the case $\alpha = 1.5$. The skewness is a consequence of long downstream (left to right) particle jumps. The peak shifts left of the mean (center of mass) at zero to balance the heavy tail on the right.

This point source solution to the fractional diffusion equation (4) has been used to model pollution in ground water [9]. The long downstream jumps result from fast velocity channels eroded through the intervening

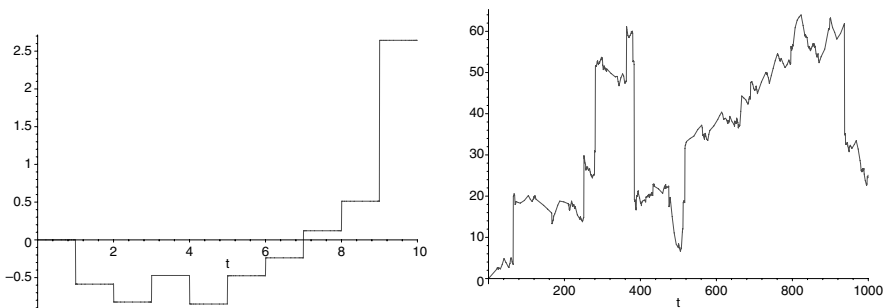


Fig. 2. A random walk with power law jumps converges to stable Lévy motion.

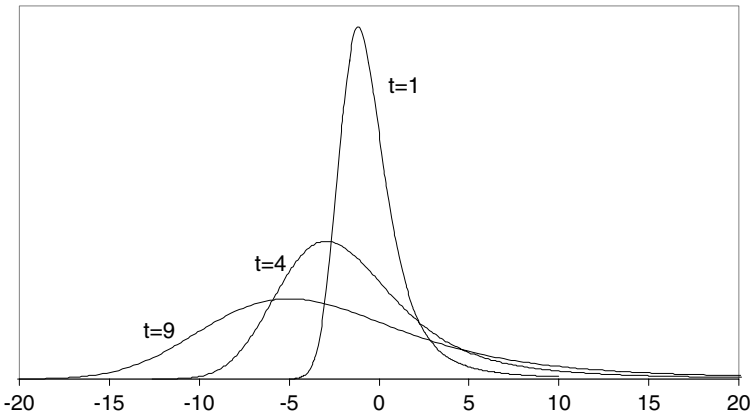


Fig. 3. Evolution of the stable Lévy motion PDF with $\alpha = 1.5$.

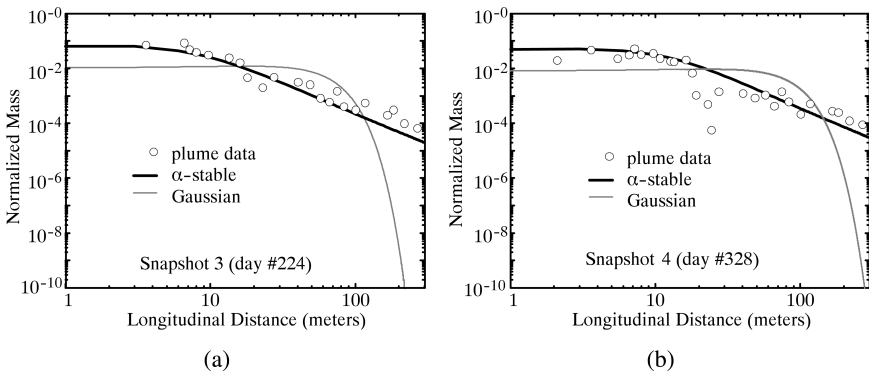


Fig. 4. FADE application to ground water pollution, from [9].

porous medium by historical flows. Figure 4 shows the best fit to measured concentrations of a tracer at the macrodispersion experimental test site (MADE site) near Columbus MS, using $\alpha = 1.1$. The log–log display illustrates the power-law right tail of the stable solution curve. The best fitting normal curve (traditional diffusion equation (4) with $\alpha = 2$) is shown for comparison. The traditional model greatly understates the risk of downstream contamination.

The intimate connection between the deterministic and random points of view is evident, once we compare the power-law jumps in the random walk model (7) to the mass transport in the fractional Fick’s law governed by

the weights (2). Both assume, as their fundamental premise, that particles travel a long distance downstream, governed by a power law.

3. Fractional Derivatives in Time

The (Caputo) fractional derivative in time can be defined, for $0 < \beta \leq 1$, as the function with Laplace transform (LT) $s^\beta \tilde{f}(s) - s^{\beta-1} f(0)$, where

$$\tilde{f}(s) = \int_0^\infty e^{-st} f(t) dt$$

is the LT of $f(t)$. When $\beta = 1$, this is the usual LT relation for the first derivative. The space-time fractional diffusion equation

$$\partial_t^\beta m(x, t) = \mathcal{D} \partial_x^\alpha m(x, t) \tag{9}$$

can be solved using Fourier–Laplace transforms (FLT) $\bar{m}(k, s)$, the FT of the LT of m . Take FLT in (9) to get $s^\beta \bar{m}(k, s) - s^{\beta-1} = \mathcal{D}(ik)^\alpha \bar{m}(k, s)$, using $\hat{m}(k, 0) = 1$, and solve to get

$$\bar{m}(k, s) = \frac{s^{\beta-1}}{s^\beta - \mathcal{D}(ik)^\alpha} = \int_0^\infty e^{u\mathcal{D}(ik)^\alpha} s^{\beta-1} e^{-us^\beta} du$$

using $\int_0^\infty e^{-au} du = 1/a$. Recognize $\hat{p}(k, u) = e^{u\mathcal{D}(ik)^\alpha}$ as the FT of the solution to the space-fractional diffusion equation $\partial_u p = \mathcal{D} \partial_x^\alpha p$. Invert the FLT to see that

$$m(x, t) = \int_0^\infty p(x, u) h(u, t) du, \tag{10}$$

where $\tilde{h}(u, s) = s^{\beta-1} e^{-us^\beta}$. The effect of the fractional time derivative is to replace the time variable in $p(x, t)$ by an operational time u governed by the function $h(u, t)$. The practical meaning, and inversion of the LT for h , will be discussed next.

In a continuous time random walk (CTRW), each particle jump X_n is preceded by a random waiting time J_n [39, 46]. Then the particle arrives at location $S(n) = X_1 + \dots + X_n$ at time $T_n = J_1 + \dots + J_n$. The spacetime random vectors (X_n, J_n) are assumed IID, and their running sum $(S(n), T_n)$ is a spacetime random walk. The CTRW is uncoupled if X_n is independent of J_n . The number of jumps by time t is $N_t = \max\{n \geq 0 : T_n \leq t\}$, so that N_t is the inverse of T_n (the graph of N_t is the graph of T_n with the axes reversed). The particle position at time t is $S(N_t)$. If $\mathbb{E}J_n = 1$, then the law of large numbers (LLN) guarantees that $N_t \sim t$ as $t \rightarrow \infty$, so the

long-time behavior of the CTRW is the same as that of a simple random walk. If $\mathbb{P}(J_n > t) \approx t^{-\beta}/\Gamma(1 - \beta)$ for some $0 < \beta < 1$ then $\mathbb{E}J_n = \infty$, and neither the CLT nor the LLN applies. A Tauberian theorem [18] shows that the PDF $w(t)$ of J has LT

$$\tilde{w}(s) = 1 - s^\beta + \dots$$

and the rescaled random walk $n^{-1/\beta}T_{[nt]}$ has FT

$$\tilde{w}(s/n^{1/\beta})^{[nt]} = \left(1 - \frac{s^\beta}{n} + \dots\right)^{[nt]} \longrightarrow e^{-ts^\beta} \quad \text{as } n \rightarrow \infty. \quad (11)$$

Inverting the LT shows that the limit is a β -stable Lévy motion D_t .

Take inverses and apply the continuous mapping theorem of probability to get $c^{-\beta}N_{ct} \approx E_t$, where the inverse process $E_t = \inf\{x > 0: D_x > t\}$ (see [27] for complete details). Then we have

$$c^{-\beta/\alpha}S(N_{ct}) = c^{-\beta/\alpha}S(c^\beta \cdot c^{-\beta}N_{ct}) \approx (c^\beta)^{-1/\alpha}S(c^\beta E_t) \approx A(E_t)$$

as the time scale $c \rightarrow \infty$, for the uncoupled CTRW.

Now we will show that the operational time $h(u, t)$ in (10) is the PDF of E_t . Note that $\{E_t \leq u\} = \{D_u \geq t\}$, as these are inverse processes. Then the PDF of E_t is

$$h(u, t) = \partial_u \mathbb{P}(E_t \leq u) = \partial_u \mathbb{P}(D_u \geq t) = \partial_u \left[1 - \int_0^t g(y, u) dy\right],$$

where $g(y, u)$ is the PDF of D_u . Use $\tilde{g}(s, u) = \exp(-us^\beta)$ from (11), and the fact that integration corresponds to dividing the LT by s , to check that

$$\tilde{h}(u, s) = \partial_u \left[1 - s^{-1}e^{-us^\beta}\right] = s^{\beta-1}e^{-us^\beta}$$

so the solution (10) to the spacetime fractional diffusion equation (9) is the PDF of $A(E_t)$, the long-time limit of a CTRW with power-law jumps $\mathbb{P}(X > x) \approx x^{-\alpha}$ and power-law waiting times $\mathbb{P}(J > t) \approx t^{-\beta}$. The form (10) comes from a conditioning argument

$$\mathbb{P}(A(E_t) = x) = \sum_u \mathbb{P}(A(u) = x | E_t = u) \mathbb{P}(E_t = u)$$

also called the law of total probability. The fractal activity time scales according to $E_{ct} \approx c^\beta E_t$ with $0 < \beta < 1$, so that operational time is slower than clock time, a sub-diffusive effect [43].

4. Vector Fractional Calculus

Vector fractional derivatives are associated with power law jumps in d -dimensional space. To understand this connection, it is useful to view the space-fractional diffusion equation as a Cauchy problem $\partial_t p = Lp$ where the space derivative operator L acts on the x variable. The form $L = \mathcal{D}_x^\alpha$ is connected with power law jumps $\mathbb{P}(X > x) \approx x^{-\alpha}$. The CTRW with these jumps, and exponential waiting times $\mathbb{P}(J > t) = e^{-\lambda t}$, is also called a compound Poisson process. Now $\mathbb{P}(N_t = n) = e^{-\lambda t}(\lambda t)^n/n!$ and

$$P(x, t) = \mathbb{P}(S(N_t) \leq x) = \sum_{n=0}^{\infty} \mathbb{P}(S(n) \leq x | N_t = n) \mathbb{P}(N_t = n)$$

by the law of total probability. Take FT to get

$$\hat{P}(k, t) = \sum_{n=0}^{\infty} \hat{f}(k)^n e^{-\lambda t} \frac{(\lambda t)^n}{n!} = e^{-\lambda t(1-\hat{f}(k))}$$

by the Taylor series for e^z , where f is the PDF of X . Clearly this solves

$$\partial_t \hat{P}(k, t) = -\lambda(1 - \hat{f}(k)) \hat{P}(k, t)$$

which inverts to the Cauchy problem

$$\partial_t P(x, t) = -\lambda P(x, t) + \lambda \int P(x - y, t) f(y) dy \tag{12}$$

using the convolution property of FT. Use the fact that $\int f(y) dy = 1$ to rewrite this in the form

$$\partial_t P(x, t) = \int (P(x - y, t) - P(x, t)) \lambda f(y) dy.$$

To arrive at the stable limit process, let $\lambda \rightarrow \infty$ and rescale the jumps: Let $X_\lambda = \lambda^{-1/\alpha} X$, with PDF $f_\lambda(y) = \lambda^{1/\alpha} f(\lambda^{1/\alpha} y)$. Using $f(y) \approx \alpha y^{-\alpha-1}/\Gamma(1 - \alpha)$ we get $\lambda f_\lambda(y) \rightarrow \alpha y^{-\alpha-1}/\Gamma(1 - \alpha)$ for all $y > 0$, so the CDF of the limit $A(t)$ solves

$$\partial_t P(x, t) = \frac{\alpha}{\Gamma(1 - \alpha)} \int_0^\infty (P(x - y, t) - P(x, t)) y^{-\alpha-1} dy. \tag{13}$$

The formula on the right-hand side is another form of the fractional derivative $\partial_x^\alpha P$. To check this, compute the FT

$$\frac{\alpha}{\Gamma(1 - \alpha)} \int_0^\infty (e^{-iky} - 1) y^{-\alpha-1} dy = (ik)^\alpha$$

for $0 < \alpha < 1$, and use the fact that $e^{-iky} \hat{P}(k, t)$ is the FT of $P(x - y, t)$. Apply ∂_x to both sides of (13) to recover the fractional diffusion equation (4) with $\mathcal{D} = 1$. The Poisson limit is an alternative to the FT argument (11), see [25] for complete details.

The balance equation (12) writes the change in probability in terms of the rate λ at which particles jump away from location x , and the rate at which particles from location $x - y$ jump to location x . This is completely analogous to the fractional Fick's law, as the proportion of particle that travels a distance y falls off like $y^{-\alpha-1}$ in both models.

More general notions of anomalous diffusion are given by the Cauchy problem $\partial_t P = LP$ with

$$Lf(x) = -v \cdot \nabla f(x) + \int_0^\infty [f(x - y) - f(x) + y \cdot \nabla f(x)] \phi(dy), \quad (14)$$

where $\phi(dy)$ is the Poisson jump intensity, and $\nabla = \partial_{x_1} + \dots + \partial_{x_d}$ is the gradient [1]. The first term adds a drift at velocity v . Taking $v = 0$ and

$$\phi(dy) = \begin{cases} a\mathcal{D} \frac{\alpha}{\Gamma(1-\alpha)} y^{-1-\alpha} dy & \text{for } y > 0 \\ b\mathcal{D} \frac{\alpha}{\Gamma(1-\alpha)} |y|^{-1-\alpha} dy & \text{for } y < 0 \end{cases}$$

in one dimension leads to $L = a\mathcal{D}\partial_x^\alpha + b\mathcal{D}\partial_{-x}^\alpha$. The negative fractional derivative ∂_{-x}^α , equivalent to multiplying the FT by $(-ik)^\alpha$, models right-to-left particle jumps. To verify $L = a\mathcal{D}\partial_x^\alpha + b\mathcal{D}\partial_{-x}^\alpha$, compute the FT

$$\frac{\alpha}{\Gamma(1-\alpha)} \int_0^\infty (e^{-iky} - 1 + ik y) y^{-\alpha-1} dy = (ik)^\alpha$$

for $1 < \alpha < 2$, see [25, p. 265]. The corresponding Cauchy problem governs the CTRW limit with $\mathbb{P}(X > x) \approx ax^{-\alpha}$ and $\mathbb{P}(X < -x) \approx bx^{-\alpha}$ so that the weights a, b balance the jumps. This version of (4) has been applied to model contamination in ground water and river flows, see [8, 12, 17]. The stable limit $A(t)$ has PDF with FT $\hat{p}(k, t) = \exp(aDt(ik)^\alpha + bDt(-ik)^\alpha)$, see [25, p. 456]. If $a = b$, this gives a model for symmetric anomalous diffusion, the case $\alpha = 1$ being the familiar Cauchy distribution.

In the vector case with $\phi(dy) = C\|y\|^{-\alpha-d}dy$ we get $L = -(-\Delta)^{\alpha/2}$ the fractional power of the Laplacian $\Delta = \nabla \cdot \nabla$, which has an interesting history [19]. The corresponding stable process in d dimensions is the limit of a random walk with power-law jumps, whose orientation is uniformly distributed over the unit sphere. If we take jumps of the form $X = R\Theta$

where $\mathbb{P}(R > r) \sim r^{-\alpha}/\Gamma(1 - \alpha)$ and Θ has an arbitrary distribution $M(d\theta)$ on the unit sphere, a Poisson limit argument yields a Cauchy problem with jump intensity $\phi(dr, d\theta) = \alpha r^{-\alpha-1} dr M(d\theta)/\Gamma(1 - \alpha)$ in polar coordinates $y = r\theta$. Compute

$$Lf(x) = -v \cdot \nabla f(x) + \int_{|\theta|=1} \mathbb{D}_\theta^\alpha f(x) M(d\theta), \tag{15}$$

where $\mathbb{D}_\theta^\alpha f(x)$ is the fractional directional derivative, equal to $\partial_r^\alpha f(x + r\theta)$ at $r = 0$, whose FT is $(ik \cdot \theta)^\alpha \hat{f}(k)$. The Cauchy problem $\partial_t p = Lp$ using (15) is called the fractional advection-dispersion equation (FADE) [23]. The FADE has found many applications in ground water hydrology [8, 9, 16], biology [3, 40], and physics [37, 38]. For example, the FADE

$$\partial_t p = v_x \partial_x p - v_y \partial_y p + \mathcal{D}_x \partial_x^\alpha + \mathcal{D}_y \partial_y^\alpha \tag{16}$$

governs anomalous diffusion with mean velocity $v = (v_x, v_y)$, the long-time limit of a vector random walk with power-law jumps in the positive x and y directions, with a probability of jumps longer than r falling off like $r^{-\alpha}$, and the proportion of x, y jumps governed by the ratio $\mathcal{D}_x/\mathcal{D}_y$.

A vector fractional calculus was developed in [30], see also [50]. Start with the vector flux $q = vp - Q\nabla p$, and write the dispersion tensor Q in terms of the distribution $M(d\theta)$ that controls jump directions:

$$Q\nabla f(x) = \int_{|\theta|=1} \theta (\theta \cdot \nabla f(x)) M(d\theta), \tag{17}$$

a mixture of directional derivatives $\mathbb{D}_\theta f(x) = \theta \cdot \nabla f(x)$ laid out in each radial direction θ according to the weights $M(d\theta)$. Together with conservation of mass $\partial_t p = \nabla \cdot q$ this leads to the traditional advection-dispersion equation (ADE) $\partial_t p = -v \cdot \nabla p + \nabla \cdot Q\nabla p$ used to model ground water contaminants [7]. Apply the FT $\hat{p}(k, t) = \int e^{-ik \cdot x} p(x, t) dx$ to get

$$\partial_t \hat{p}(k, t) = -v(ik) \hat{p}(k, t) + (ik) \cdot Q(ik) \hat{p}(k, t)$$

whose point source solution $\hat{p}(k, t) = \exp(-tv(ik) + (ik) \cdot tQ(ik))$ inverts to a multivariable Gaussian PDF with mean tv and covariance matrix $2tQ$. The FADE comes from a fractional vector flux $q = vp - \nabla_M^{\alpha-1} p$ where the fractional gradient

$$\nabla_M^{\alpha-1} f(x) = \int_{|\theta|=1} \theta \mathbb{D}_\theta^{\alpha-1} f(x) M(d\theta)$$

is a mixture of fractional directional derivatives. Use FT to check that

$$\nabla \cdot \nabla_M^{\alpha-1} f(x) = \int_{|\theta|=1} \mathbb{D}_\theta^\alpha f(x) M(d\theta).$$

These same ideas can be used to extend the divergence, curl, and basic theorems of vector calculus (divergence theorem, Stokes theorem) to a fractional form [30]. Time-fractional Cauchy problems are considered in [1, 5, 21, 35].

5. Multi-Scaling Fractional Derivatives

There is no reason why the order of the space-fractional derivative in the FADE (16) should be the same in both coordinates. An extended model uses matrix scaling. Consider a random walk with jumps $X = R^E \Theta$ where $\mathbb{P}(R > r) \approx r^{-1}$ and Θ has an arbitrary distribution $M(d\theta)$ on the unit sphere. The matrix power $R^E = \exp(E \log R)$ where the matrix exponential $\exp(A) = I + A + A^2/2 + \dots$ as usual. If $E = \text{diag}(1/\alpha_1, \dots, 1/\alpha_d)$ a diagonal matrix, then $R^E = \text{diag}(R_1, \dots, R_d)$ with $\mathbb{P}(R_i > r) \approx r^{-\alpha_i}$, allowing a different tail index in each coordinate. For a CTRW with these jumps, and exponential waiting times, a Poisson limit argument shows that the CTRW converges to a vector-valued process $A(t)$ with operator scaling $A(ct) \approx c^E A(t)$ [24, 47]. The limit process $A(t)$ is called an operator stable Lévy motion [25]. Its density $p(x, t)$ solves the Cauchy problem $\partial_t P = LP$ with generator L given by (14), and jump intensity $\phi(dy) = r^{-2} dr M(d\theta)$ in the multi-scaling polar coordinates $y = r^E \theta$ [20, 25, 47]. For example, the multi-scaling FADE

$$\partial_t p = -v_x \partial_x p - v_y \partial_y p + \mathcal{D}_x \partial_x^{\alpha_x} + \mathcal{D}_y \partial_y^{\alpha_y} \tag{18}$$

governs the long-time limit of a vector random walk with power-law jumps $R^E \Theta = (X, Y)$, with exponent $E = \text{diag}(1/\alpha_x, 1/\alpha_y)$, and Θ points in the x, y directions with probability proportional to $\mathcal{D}_x, \mathcal{D}_y$, respectively. Then $\mathbb{P}(X > r) \approx r^{-\alpha_x}$ and $\mathbb{P}(Y > r) \approx r^{-\alpha_y}$ so that each fractional derivative codes power law jumps in the corresponding coordinate direction.

By varying the matrix exponent E and the distribution of the jump angle Θ , a wide variety of models can be constructed. Eigenvectors of E determine the coordinate system, the corresponding eigenvalues code the power law tails (order of the fractional derivative) in each coordinate, and Θ directs the jumps. Practical details are laid out in [26]. The multi-scaling FADE has been applied to ground water pollution in granular

aquifers [41, 47, 52] and fractured rock [44], tick-by-tick stock data [29], and chaotic dynamics of microbes in anisotropic porous media [42].

6. Simulation

Numerical solutions to (4) are developed in [28, 31, 48] based on a shifted version of the finite difference $\Delta^\alpha f(x) = \sum_{m=0}^\infty w_m f(x - mh + h)$. The shift is necessary for numerical stability, even in the case $\alpha = 2$. Numerical methods for the vector equation (18) are developed in [32, 49] based on operator splitting: In one step of the iteration, the $\partial_x^{\alpha_x}$ term is applied while y is held constant, and vice versa. An application in [3] considers a fractional reaction-dispersion equation that models an invasive species crossing a barrier:

$$\partial_t p = C\partial_x^\alpha p + D\partial_y^2 p + rp \left(1 - \frac{p}{K}\right),$$

where population density $p(x, y, t)$, r is the intrinsic growth rate of the species, and K is the environmental carrying capacity [33]. Figure 5 shows the numerical solution, via operator splitting of the reaction and dispersion terms. In the classical model $\alpha = 2$ (top), the invading species leaks slowly

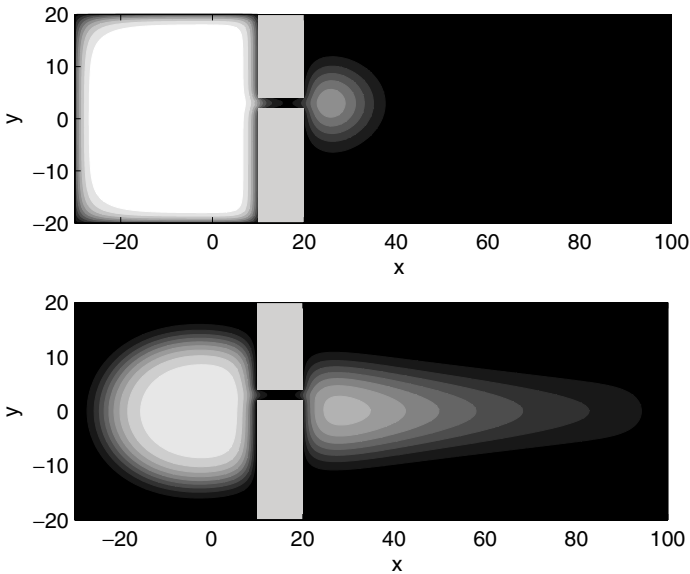


Fig. 5. Fractional model for invasive species crossing a barrier, from [3].

through the slit barrier. In the fractional model $\alpha = 1.7$ (bottom) the invaders jump the barrier, and the slit is irrelevant. This demonstrates the effect of a nonlocal fractional derivative as a model for long jumps, and its implications for applications in ecology. The fractional derivative is relevant in such problems, since many ecological studies have documented heavy tail dispersal kernels (distance between parent and offspring) in ecological applications [3].

A finite difference approximation to the multi-scaling fractional derivative was considered in [2], but for most practical applications, it seems easier to use particle tracking [22]. A random walk with jumps $X = R^E\Theta$ faithfully approximates the operator stable process $A(t)$, and a histogram of particles estimates the PDF $p(x, t)$ that solves the multi-scaling FADE, see [52]. Figure 6 illustrates the particle tracking solution in the case $v_x = 10$, $v_y = 0$ (left-to-right flow), $\alpha_x = 1.5$, and $\alpha_y = 1.9$ (more anomalous dispersion in the direction of flow). The jump directions and respective weights are illustrated in the upper right inset. Dots are individual particles, and continuous curves are the corresponding solution via inverse fast Fourier transform (FFT) of $\hat{p}(k, t)$. The FFT method is only viable for constant coefficients.

A more sophisticated simulation method that preserves the exact location and timing of the large jumps was recently developed [14] based on a shot noise representation $X = R^E\Theta$ for the large jumps, and a Brownian motion approximation for the small jumps (there are infinitely many of those). The same idea was used in [13] for the vector stable process

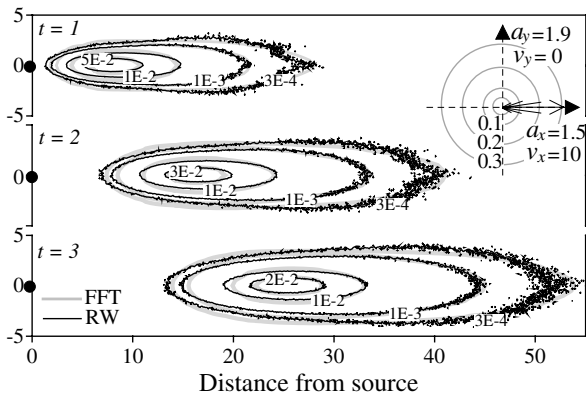


Fig. 6. Particle tracking solution of the multi-scaling FADE (18) from [52].

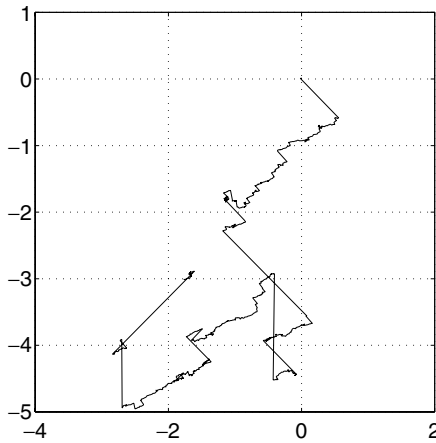


Fig. 7. Particle motion behind the multi-FADE (18) for flow in fractured rock.

that underlies the FADE. Figure 7 shows the resulting particle motion for an application to flow in fractured rock. In this example, transport model number 22 from [44], E has eigenvectors at $+45^\circ$ and -45° with eigenvalues $b_1 = 1/1.1$ and $b_2 = 1/1.2$ respectively. Θ points to $\pm 45^\circ$ with probability 0.4, and 90° with probability 0.2. The graph shows particle location in a moving coordinate system with origin at the plume center of mass. The Θ directions model fracture orientation, the Θ weights determine the proportion of transport events in each fracture direction, and the eigenvalues of E determine the length of power-law particle jumps. The $\Theta = 90^\circ$ jumps are a blend of two power laws according to $X = R^E \Theta$.

7. Tempered Fractional Derivatives

Tempering cools the longest jumps in a power law PDF, so that all moments exist. Tempered diffusion models transition from fractional behavior at early time to traditional diffusion at late time, a kind of transient anomalous diffusion. This transition is widely observed in practice, for example, as a basic “stylized fact” in mathematical finance [15]. For applications to geophysics, see [34]. The stable PDF $f(t)$ behind the time-fractional diffusion equation (9) has LT $\hat{f}(s) = e^{-s^\beta}$. The exponentially tempered version $f(t)e^{-\lambda t}$ integrates to $e^{-\lambda^\beta}$ by the LT formula, so that $f_\lambda(t) = f(t)e^{-\lambda t}e^{\lambda^\beta}$ is a valid PDF on $t > 0$, called the tempered stable. For small $\lambda > 0$ it behaves like the stable PDF until t is large, after which exponential tempering takes

over. Compute

$$\tilde{f}_\lambda(s) = \int_0^\infty e^{-st} f(t) e^{-\lambda t} e^{\lambda^\beta} dt = e^{-[(\lambda+s)^\beta - \lambda^\beta]}$$

which reduces to the stable LT as $\lambda \rightarrow 0$. Similarly, the stable PDF with FT $\hat{p}(k, t) = \exp(t\mathcal{D}(ik)^\alpha)$ from the space-fractional diffusion equation (4) has a tempered version with FT $\hat{p}_\lambda(k, t) = \exp(t\mathcal{D}[(\lambda + ik)^\alpha - \lambda^\alpha])$. The tempered derivative $\partial_x^{\beta, \lambda} g(x)$ is the inverse FT of $[(\lambda + ik)^\alpha - \lambda^\alpha] \hat{g}(k)$. Invert this FT, using the fact that $\tilde{g}(s - \lambda)$ is the FT of $e^{\lambda t} g(t)$ (twice), to see that

$$\partial_x^{\alpha, \lambda} g(x) = e^{-\lambda x} \partial_x^\alpha (e^{\lambda x} g(x)) - \lambda^\alpha g(x).$$

The PDF $p_\lambda(x, t)$ of the tempered stable process $A_\lambda(x)$ solves the tempered fractional diffusion equation [6, 10]

$$\partial_t p(x, t) = \mathcal{D} \partial_x^{\alpha, \lambda} p(x, t) \quad (19)$$

and transitions from stable PDF to Gaussian PDF as $t \rightarrow \infty$. The random walk model behind this tempered anomalous diffusion is laid out in [11]: For each particle jump, an independent exponential with rate λ is drawn, and the smaller of the two applies. See [34] for the tempered time-fractional diffusion model.

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