Models of space-fractional diffusion: a critical review

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Abstract

Space-fractional diffusion problems are investigated from the modeling point of view. It is pointed out that the elementwise power of the Laplacian operator in $\mathbb{R}^n$ is an inadequate model of fractional diffusion. Also, the approach with fractional calculus using zero extension is not a proper model of homogeneous Dirichlet boundary conditions. At the time, the spectral definition of the fractional Dirichlet Laplacian seems to be in many aspects a proper model of fractional diffusion.

Keywords: fractional-order diffusion, fractional calculus, fractional Laplacian, modeling

1. Introduction

The accurate measurement techniques in the last decades confirmed the occurrence of the space-fractional (or anomalous) diffusion in a wide range of real-life phenomena. By tracking individual particles, it is possible to estimate their average displacement $\langle |s(t)|\rangle$ over a short time interval $(0, t)$. While in a standard diffusion process the linear dependence $\langle |s(t)|\rangle \sim t^{\frac{1}{2}}$ is valid, in many cases, the proportionality $\langle |s(t)|\rangle \sim t^{\frac{\alpha}{2}}$ or $\langle |s(t)|^2\rangle \sim t^{\alpha}$ can be detected with $\alpha \neq 1$. In a probabilistic interpretation, the random displacement represents an α-stable Lévy process [1] so that $s(t)$ is distributed with some t-dependent density.

Also, a number of continuous deterministic models have been proposed, where the non-local spatial operators were associated with the anomalous diffusion. Based on these, various numerical methods were developed started with the works in [2] and [3]. A critical point of all PDE models is to incorporate and use boundary conditions. From the point of view of the functional analysis, they are already necessary to define the differential operators. In many real situations, one should use Neumann boundary conditions in the models. A corresponding analysis can be found in [4] and [5].

In the literature, mostly problems with homogeneous Dirichlet boundary conditions were investigated; a systematic study of incorporating inhomogeneous data has just been started [6]. The aim of this contribution is to give an overview of these approaches from the point of view how realistic models they deliver for the anomalous diffusion. Therefore, we focus on the multidimensional models.

2. Mathematical preliminaries: basic models for anomalous diffusion

Differential operators corresponding to the diffusion will be defined on a Lipschitz domain $\Omega \subset \mathbb{R}^d$. They are all non-local in the sense that the flux at a given point $\mathbf{x}$ depends on the density function in a neighborhood of $\mathbf{x}$. For $\Omega = \mathbb{R}^d$, they can be defined on the Schwartz space of rapidly decreasing functions. Usually, we do not give explicitly the largest linear space where these operators are defined. In each case, the positive constant $\frac{\alpha}{2}$ denotes the exponent of the classical diffusion operator, where in all cases $\alpha \in (0, 2]$.

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For a bounded interval $(a, b) = \Omega$, the most popular choice is the symmetric Riemann–Liouville derivative $\partial_{\mathrm{RL}}^{\alpha}$, which is defined for $1 < \alpha < 2$ with

$$\partial_{\mathrm{RL}}^{\alpha} u(x) = \frac{1}{2\Gamma(2-\alpha)} \partial^2 \left\{ x \to \int_a^x u(s)(x-s)^{1-\alpha} \, \mathrm{d}s + \int_x^b u(s)(s-x)^{1-\alpha} \, \mathrm{d}s \right\}. \tag{1}$$

Another frequently used definition (for $1 < \alpha < 2$ and $u \in C^2[a, b]$) was suggested by Caputo:

$$\partial_{\mathrm{C}}^{\alpha} u(x) = \frac{1}{2\Gamma(2-\alpha)} \int_a^x u"(s)(x-s)^{1-\alpha} \, \mathrm{d}s + \int_x^b u"(s)(s-x)^{1-\alpha} \, \mathrm{d}s. \tag{2}$$

This definition can be used, *e.g.*, directly in a model of neuronal transmission [7]. For the relation of (1) and (2), we refer to [8], Theorem 2.7.

Based on the classical theory of fractional order derivatives [9], a number of alternative definitions are available, which are, in general, not equivalent. For a clear overview on these, we refer to [8] and [10].

For $\Omega = \mathbb{R}$, many of the different definitions coincide [11]. We mention three of them, which are linked to the operators in this section. The spectral definition of the fractional Laplacian reads as

$$(-\Delta)^{\frac{\alpha}{2}} u = \mathcal{F}^{-1}(|\mathtt{Id}|^{\alpha} \mathcal{F} u), \tag{3}$$

where $\mathcal{F}$ denotes the Fourier transform and $\mathtt{Id}$ the identity function. The following definition was proposed by M. Riesz

$$\partial_{\mathrm{R}}^{\alpha} u(x) = -\frac{1}{2\Gamma(2-\alpha)\cos(\alpha\pi/2)} \partial^2 \left\{ x \to \int_{-\infty}^x u(s)(x-s)^{1-\alpha} \, \mathrm{d}s + \int_x^{\infty} u(s)(s-x)^{1-\alpha} \, \mathrm{d}s \right\}, \tag{4}$$

which is a generalization of (1). For its definition domain, we refer to [5].
As a third one, we mention Balakrishnan's definition:

$$(-\Delta)^{\frac{\alpha}{2}} u = \frac{\sin \alpha\pi/2}{\pi} \int_0^{\infty} \Delta(s \cdot \mathtt{Id} - \Delta)^{-1} u \cdot s^{\alpha/2-1} \, \mathrm{d}s,$$

which applied for the sin function with the well-known identity $\int_0^{\infty} \frac{s^{\alpha/2-1}}{s+1} \, \mathrm{d}s = \frac{\pi}{\sin(\alpha\pi/2)}$ (see, [12], 3.222) gives

$$(-\Delta)^{\frac{\alpha}{2}} \sin = \frac{\sin(\alpha\pi/2)}{\pi} \int_0^{\infty} \sin \cdot \frac{1}{s+1} \cdot s^{\alpha/2-1} \, \mathrm{d}s = \sin.$$

Therefore, we have the following identities for the trigonometric functions:

$$(-\Delta)^{\frac{\alpha}{2}} \sin = \partial_{\mathrm{R}}^{\alpha} \sin = \sin \qquad \text{and} \qquad (-\Delta)^{\frac{\alpha}{2}} \cos = \partial_{\mathrm{R}}^{\alpha} \cos = \cos. \tag{5}$$

For $\Omega = \mathbb{R}^d$, the spectral definition in (3) can be applied without any change.
For $d = 2$ the alternative definition

$$\partial_{\mathrm{RL},2}^{\alpha} u(x, y) = \partial_{x,\mathrm{R}}^{\alpha} u(x, y) + \partial_{y,\mathrm{R}}^{\alpha} u(x, y) \tag{6}$$

is used frequently in the literature in space-fractional diffusion problems [13], [14]. Many authors apply this operator to solve numerically related problems, such as the Schrödinger equation [15] and reaction-(sub)diffusion equations [16].

For a bounded $\Omega \subset \mathbb{R}^d$ with homogeneous Dirichlet boundary conditions, the spectral definition can again be applied similarly to the one in (3):

$$(-\Delta_{\mathcal{D}})^{\frac{\alpha}{2}} u = \sum_{j=1}^{\infty} \lambda_j^{\frac{\alpha}{2}} f_j, \tag{7}$$

where $\{\lambda_j\}_{j\in\mathbb{N}^+}$ and $\{f_j\}_{j\in\mathbb{N}^+}$ denote the eigenvalues and the eigenfunctions, respectively, of the positive self-adjoint operator $-\Delta_{\mathcal{D}}$, the opposite of the Dirichlet Laplacian.

Another approach to incorporate homogeneous Dirichlet boundary conditions is offered by the model

$$\begin{cases} \partial_t u(t,\mathbf{x}) = -(-\Delta)^{\frac{\alpha}{2}} u(t,\mathbf{x}) & t\in(0,T),\ \mathbf{x}\in\Omega \\ u(t,\mathbf{x}) = 0 & t\in(0,T),\ \mathbf{x}\in\Omega^c \\ u(0,\mathbf{x}) = u_0 & \mathbf{x}\in\Omega \end{cases} \tag{8}$$

with a given initial function u_0. In practice, we apply the fractional Laplacian to the zero-extension of a function u defined on Ω with homogeneous Dirichlet boundary data and consider its restriction to Ω. The spatial differential operator in (8) is a special case of the non-local differential operators analyzed in [17] and recently, for time-dependent problems in [18]. This setting shows clearly that for non-local differential operators, initial or boundary data should be given also outside of the computational domain Ω. For a spectral comparison of the spatial operator in (8) with the one in (7), we refer to [19].

An important building block of the models and the corresponding numerical approximations is the notion of fluxes. In the framework of the non-local analysis, this is also non-local so that it is defined between different subdomains. In the one-dimensional case, however, one can identify the flux $\Psi_\alpha[u]$ (corresponding to the exponent α and the density $u\in L_{1,\mathrm{loc}}$) between $(-\infty,b)$ and (b,∞) with $\Psi_\alpha[u](b)$. Note that the flux (indeed, a flux density) crossing a point is a physical quantity so that in any meaningful linear model there should exist a flux function satisfying the following conditions:

(i) Ψ_α is translation invariant, i.e. for $u_s:\mathbb{R}\to\mathbb{R}$ with $u_s(y)=u(y-s)$ we have $\Psi_\alpha[u_s](y+s)=\Psi_\alpha[u](y)$.

(ii) Ψ_α is antisymmetric, i.e. for $u^\circ:\mathbb{R}\to\mathbb{R}$ with $u^\circ(y)=u(-y)$ we have $\Psi_\alpha[u^\circ](0)=-\Psi_\alpha[u](0)$.

(iii) Ψ_α is linear: for all $u,v\in L_{1,\mathrm{loc}}$ and $\lambda,\mu,b\in\mathbb{R}$ we have $\Psi_\alpha[\lambda u+\mu v](b)=\lambda\Psi_\alpha[u](b)+\mu\Psi_\alpha[u](b)$.

Remark: The relation in (ii) is explicitly stated in [20] for the flux between $(-\infty,b)$ and (b,∞).

3. Results

For a bounded interval $(a,b)=\Omega$ both the symmetric Riemann–Liouville and the Caputo derivative can be used for modeling fractional diffusion. For any anisotropic phenomena, it is essential that this symmetric version is used. Accordingly, in the theory it is pointed out the left-integral is the adjoint of the right-integral if homogeneous boundary conditions are applied [3], [21].

For $\Omega=\mathbb{R}$, as mentioned, many of the fractional differential operators coincide such that we can not distinguish between the different models.

For $\Omega=\mathbb{R}^d$, we point out that the differential operator $\partial^\alpha_{\mathrm{GL}}$ is not appropriate if rotational invariance should be assumed in a model.

Theorem 1. *The operator $\partial^\alpha_{RL,2}$ is not rotation invariant; i.e. one can find a smooth function $u:\mathbb{R}^2\to\mathbb{R}$ and a rotation $B:\mathbb{R}^2\to\mathbb{R}^2$ with $B(x,y)=(\xi,\zeta)$ such that*

$$\partial^\alpha_{RL,2}u(x,y)\neq\partial^\alpha_{RL,2}u(B^{-1}(\xi,\zeta)).$$

Proof: We give u and B with $u(x,y)=\sin x\sin y$ and $B(x,y)=\left(\frac{x+y}{\sqrt{2}},\frac{x-y}{\sqrt{2}}\right)$, respectively. Using (5), a simple calculation shows that

$$\partial^\alpha_{\mathrm{RL},2}u(\frac{\pi}{2},\frac{\pi}{2})=\partial^\alpha_{\mathrm{R}}u(\cdot,\frac{\pi}{2})|_{\frac{\pi}{2}}+\partial^\alpha_{\mathrm{R}}u(\frac{\pi}{2},\cdot)|_{\frac{\pi}{2}}=\partial^\alpha_{\mathrm{R}}\sin|_{\frac{\pi}{2}}+\partial^\alpha_{\mathrm{R}}\sin|_{\frac{\pi}{2}}=\sin\frac{\pi}{2}+\sin\frac{\pi}{2}=2.$$

On the other hand, taking the new variables $\eta = \frac{x-y}{\sqrt{2}}$ and $\xi = \frac{x+y}{\sqrt{2}}$, which corresponds to a rotation with the angle $-\frac{\pi}{4}$, the function u can be given as

$$u(\xi,\eta) = \sin\frac{\xi+\eta}{\sqrt{2}}\sin\frac{\xi-\eta}{\sqrt{2}} = \frac{1}{2}(\cos\sqrt{2}\eta - \cos\sqrt{2}\xi). \tag{9}$$

Also, we rewrite the point with $x = \frac{\pi}{2}$ and $y = \frac{\pi}{2}$ as $\xi = \frac{\pi}{\sqrt{2}}$ and $\eta = 0$ with the new variables. Therefore, with the aid of (5) and (9) we have

$$\partial^\alpha_{\mathrm{RL},2} u(\frac{\pi}{\sqrt{2}},0) = \frac{1}{2}(\partial^\alpha_{\mathrm{RL}}\cos\sqrt{2}\eta|_0 - \partial^\alpha_{\mathrm{RL}}\cos\sqrt{2}\xi|_{\frac{\pi}{\sqrt{2}}}) = \frac{\sqrt{2}^\alpha}{2}(\cos 0 - \cos\pi) = \sqrt{2}^\alpha$$

with respect to the new variables, which coincides with 2 if and only if $\alpha = 2$. □

This shows that the two-dimensional Riesz derivative $\partial^\alpha_{\mathrm{RL},2}$ depends on choice of the coordinate system, such that it is not appropriate for modeling any kind of isotropic diffusion. If anisotropic fractional diffusion is assumed, an appropriate differential operator can be the one in [22], which is a directionally weighted form of the fractional Laplacian.

For a bounded $\Omega \subset \mathbb{R}^d$ we investigate the non-local approach. Using assumptions (i)-(iii) for the flux, we point out that the model in (8) fails to satisfy a basic requirement of the PDE models.

Theorem 2. *The flux* Ψ_α *in* (8) *does not depend continuously on* α*.*

Proof: We first determine the initial flux in the following standard diffusion problem:

$$\begin{cases} \partial_t u(t,x) = \Delta_{\mathcal{D}} u(t,x) & t \in (0,T),\ x \in (0,\pi) \\ u(0,x) = \sin x & x \in (0,\pi). \end{cases} \tag{10}$$

According to Fick's first law, the flux at $x = \pi$ should be -1. To make a link with (8), we note that u and the corresponding flux can be obtained by the restriction $\tilde{u}|_{(0,\pi)}$, where $\tilde{u}$ is the solution of the extended problem:

$$\begin{cases} \partial_t \tilde{u}(t,x) = \Delta\tilde{u}(t,x) & t \in (0,T),\ x \in \mathbb{R} \\ \tilde{u}(0,x) = \sin x & x \in \mathbb{R}, \end{cases} \tag{11}$$

In this sense, we have that

$$\Psi_2(\sin)(\pi) = -1. \tag{12}$$

Using (i), (ii), (iii) and (i) again, we obtain for the flux Ψ_α corresponding to the exponent $\frac{\alpha}{2}$ the following:

$$\Psi_\alpha(\chi_{[0,\pi]}\cdot\sin)(\pi) = \Psi_\alpha(\chi_{[-\pi,0]}\cdot(-\sin))(0) = -\Psi_\alpha(\chi_{[0,\pi]}\cdot\sin)(0) = \Psi_\alpha(\chi_{[0,\pi]}\cdot(-\sin))(0) = \Psi_\alpha(\chi_{[\pi,2\pi]}\cdot\sin)(\pi).$$

Taking the sum of first and the last terms and using the linearity, we get

$$\Psi_\alpha(\chi_{[0,\pi]}\cdot\sin)(\pi) = \frac{1}{2}\Psi_\alpha(\chi_{[0,2\pi]}\cdot\sin)(\pi)$$

such that in case of continuity of the flux, using the locality of Ψ_2 and (12) we had

$$\lim_{\alpha\to 2}\Psi_\alpha(\chi_{[0,\pi]}\cdot\sin)(\pi) = \frac{1}{2}\Psi_2(\chi_{[0,2\pi]}\cdot\sin)(\pi) = -\frac{1}{2}.$$

This differs, however, from the flux in (12). □

Remark: We still think that non-local analysis in [20] is a proper tool for modeling anomalous diffusion but the zero extension in (8) does not correspond to the Dirichlet boundary conditions. Instead, in the one-dimensional case, one should apply the extension in [5].

In light of the above analysis, we suggest in each case the spectral definition given in (3) and (7). This has also the following favorable properties:

- The models in (3) and (7) do not depend on the spatial dimension or on the geometry of the domain.
- In a microscopic view, the true model of the fractional order diffusion is a fractional order Brownian random walk, and applying homogeneous Dirichlet conditions corresponds to the absorbing boundary condition. The infinitesimal generator of such a stochastic process is even $-(-\Delta_{\mathcal{D}})^{\frac{\alpha}{2}}$, see [1].
- The operator $-(-\Delta)^{\frac{\alpha}{2}}$ on $\mathbb{R}^d$ is rotation invariant, see [23].
- For any $u_0 \in$ the problem
$$\begin{cases} \partial_t u(t,\mathbf{x}) = \Delta_{\mathcal{D}} u(t,\mathbf{x}) & t \in (0,T),\ \mathbf{x} \in \Omega \\ u(0,\mathbf{x}) = u_0(\mathbf{x}) & \mathbf{x} \in \Omega \end{cases}$$
is well-posed and the solution $u(t,\cdot) : \Omega \to \mathbb{R}$ is smooth, see [24]. For a generalization, we refer to [25].

For a detailed discussion of this approach with further real applications and analysis, we refer to the monograph [26].

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