Super-diffusion and space fractional pde

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Motivation

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Strange behaviour – albatrosses fly by the rules of anomalous diffusion

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Edited* by Jennifer Lippincott-Sc

Diffusion in the plasma mem
display anomalous dynamics
this diffusion pattern remain

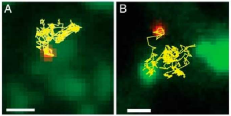


Fig. 1. Overlay image of GFP-tagged Kv2.1 clusters and individual QDs. Kv2.1 clusters are shown in green and QD-tagged channels in red. The trajectories of (*A*) a clustered and (*B*) a nonclustered (free) Kv2.1 channels are shown. Interestingly, the nonclustered channel ignores the compartment perimeters and the channel travels freely into and out of a cluster. Scale bars: 1 μm.

- super-diffusion: mass spreading with ∞ second moment
- observations incompatible with finite 2nd moment [Metzler+ Klafter, (2004)][Clark, Silman, Kern, Macklin, HilleRisLambers, (1999)
- tracer tests in rivers: tracer density measured [Deng, Singh Bengtsson, (2004)][Benson, Schumer, Meerschaert, Wheatcraft (2001)]

- animal, seeds: sometimes tracer density sometimes individual trajectories
- polymers in biological membranes
- water molecules in porous media [Néel, Bauer, Fleury,(2014)]

Organisation

- 1. Space fractional diffusion equations
- 2. Fractional integrals and derivatives
- 3. 1D stable Lévy motion
- 4. Stable Lévy motion in higher dimension
- 5. Space fractional diffusion equation : stable Lévy motion density, boundary conditions

1. Space fractional diffusion equation

1.1. Definition

- in 1D: $\partial_t C = \partial_x[-uC] + D[p\frac{\partial^\alpha C}{\partial_+ x^\alpha} + (1-p)\frac{\partial^\alpha C}{\partial_- x^\alpha}]$
- in 2D:
$\frac{\partial C}{\partial t}(\mathbf{x},\ t) + \boldsymbol{\nabla}\cdot\mathbf{u}(\mathbf{x},\ t)C(\mathbf{x},\ t) = \boldsymbol{\nabla}\cdot\overline{\overline{\mathbf{D}}}\nabla_{\boldsymbol{p}}^{\boldsymbol{\alpha}-\mathbf{1}}C(\mathbf{x},\ t) + S_c(\mathbf{x},\ t)$
- $\nabla_{\boldsymbol{p}}^{\boldsymbol{\alpha}-\mathbf{1}}C \equiv \begin{pmatrix} p_1\frac{\partial^{\alpha_1-1}C}{\partial_+ x_1^{\alpha_1-1}} + (1-p_1)\frac{\partial^{\alpha_1-1}C}{\partial_- x_1^{\alpha_1-1}} \\ p_2\frac{\partial^{\alpha_2-1}C}{\partial_+ x_2^{\alpha_2-1}} + (1-p_2)\frac{\partial^{\alpha_2-1}C}{\partial_- x_2^{\alpha_2-1}} \end{pmatrix}$
- provided derivatives exist: $\frac{\partial}{\partial x}\frac{\partial^{\alpha_1-1}C}{\partial_+ x^{\alpha_1-1}} = \frac{\partial^\alpha C}{\partial_+ x^\alpha}$
- Meerschaert+Sikorskii (2012)]

1.2. Normal diffusion: a particular case

- in 1D: $\partial_t C = \partial_x[-uC] + D[p\frac{\partial^2 C}{\partial_+ x^2} + (1-p)\frac{\partial^2 C}{\partial_- x^2}]$
- in 2D:
  $\frac{\partial C}{\partial t}(\mathbf{x},\ t) + \boldsymbol{\nabla} \cdot \mathbf{u}(\mathbf{x},\ t)C(\mathbf{x},\ t) = \boldsymbol{\nabla} \cdot \overline{\overline{\mathbf{D}}}\nabla^{\mathbf{1}}_{\boldsymbol{p}} C(\mathbf{x},\ t) + S_c(\mathbf{x},\ t)$
- $\nabla^{\mathbf{1}}_{\boldsymbol{p}} C \equiv \begin{pmatrix} \frac{\partial C}{\partial x_1} \\ \frac{\partial C}{\partial x_2} \end{pmatrix}$

2. Fractional integral/derivative

2.1. Definitions

Riemann-Liouville derivatives in $]a, b[$:

$\frac{\partial^{\alpha'} f}{\partial_+ x^{\alpha'}}(x) = \frac{\partial}{\partial x}(I_{+x}^{1-\alpha'} f)(x)$

$\frac{\partial^{\alpha'} f}{\partial_- x^{\alpha'}}(x) = -\frac{\partial}{\partial x}(I_{-x}^{1-\alpha'} f)(x)$

$\alpha' \in]0, 1]$

Riemann-Liouville integrals $I_{+,x}^{\gamma}$ and I_{-x}^{γ} in $]a, b[$:

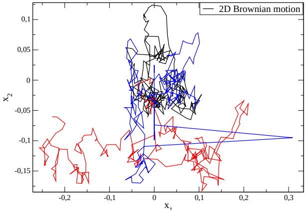
$I_{+,x}^{\gamma} f(x) = \frac{1}{\Gamma(\gamma)} \int_a^x \frac{f(x')}{(x-x')^{\gamma-1}} dx'$ and $I_{-,x}^{\gamma} f(x) = \frac{1}{\Gamma(\gamma)} \int_x^b \frac{f(x')}{(x'-x)^{\gamma-1}} dx'$

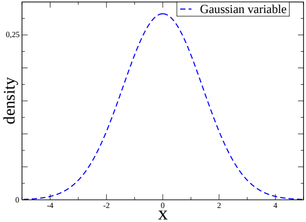
2.2. Fourier transform

- 1D: $\hat{f}(k) = \int_{-\infty}^{+\infty} e^{ikx} f(x) dx$
- derivative: $\frac{\partial f}{\partial x}$: $-ik\hat{f}(k)$
- $\frac{\partial^\alpha f}{\partial_+ x^\alpha}$: $(-ik)^\alpha \hat{f}(k)$
- $\frac{\partial^\alpha f}{\partial_- x^\alpha}$: $(ik)^\alpha \hat{f}(k)$

3. Diffusion equation and Brownian motion

3.1. Brownian motion





- in 1D or more
- $\mathbf{B}(t)$: independent increments
- $d\mathbf{B}([t, t+dt[) \overset{d}{=} (2dt)^{1/2}\mathbf{G}$
- $\mathbf{G}$:standard centered gaussian random variable of $\mathbb{R}^d$

3.2. From Brownian motion to diffusion equation

1D: $dX([t, t+dt[) = u(X(t))dt + D^{1/2} dB([t, t+dt[)$

2D: $d\mathbf{X}([t, t+dt[) = \mathbf{u}(\mathbf{X}(t))dt + \begin{pmatrix} D_{11}^{1/2} & 0 \\ 0 & D_{22}^{1/2} \end{pmatrix} d\mathbf{B}([t, t+dt[)$

the probability density function C: $\frac{\partial C}{\partial t}(\mathbf{x},\ t) + \boldsymbol{\nabla} \cdot \mathbf{u}(\mathbf{x},\ t) C(\mathbf{x},\ t)$

$= \boldsymbol{\nabla} \cdot \overline{\overline{\mathbf{D}}} \nabla_{\boldsymbol{p}}^{\mathbf{1}} C(\mathbf{x},\ t)$, $\nabla_{\boldsymbol{p}}^{\mathbf{1}} C \equiv \frac{\partial C}{\partial x}$ in 1D

$\nabla_{\boldsymbol{p}}^{\mathbf{1}} C \equiv \left(\frac{\partial C}{\partial x_1}, \frac{\partial C}{\partial x_2} \right)^T$ in 2D

4. More general stable Lévy motion

4.1. Replace BM by stable motion, in 1D

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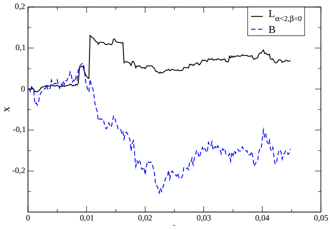
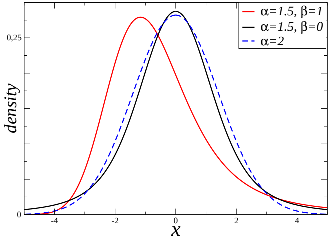
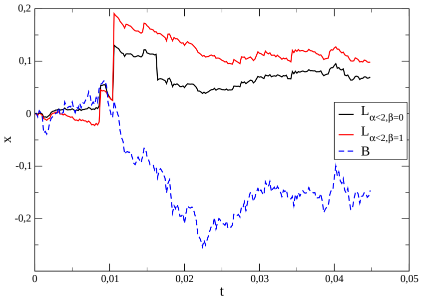




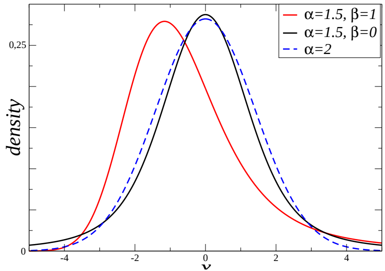
- $dX([t, t+dt[) = u(X(t)dt + D^{1/\alpha} dL_{\alpha,\beta}([t, t+dt[)$ and $X(0)$: process of p.d.f C solution of $\partial_t C = \partial_x[-uC] + D[p\frac{\partial^\alpha C}{\partial_+ x^\alpha} + (1-p)\frac{\partial^\alpha C}{\partial_- x^\alpha}]$ with $\beta = 2p - 1$
- $dL_{\alpha,\beta}([t, t+dt[)$ independent of the past as $d\mathbf{B}([t, t+dt[)$
- $dL_{\alpha,\beta}([t, t+dt[) \stackrel{d}{=} -dt^{1/\alpha} \cos\frac{\pi\alpha}{2} S(\alpha, \beta)$
- $S(\alpha, \beta)$ stable 1D random variable
- $S(2, \beta)$ 1D gaussian random variable

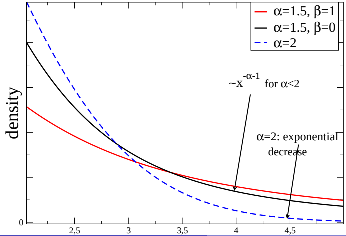
4.1. 1D stable process



- stable process
  $\alpha < 2$: more very large jumps than $\alpha = 2$
- $\beta > 0$ and $\alpha < 2$: larger large jumps
- $\beta > 0$ and $\alpha < 2$: jumps of moderate size made smaller

4.2. Stable RV





- stable random variable $S(\alpha, \beta)$, stability exponent $0 < \alpha \leq 2$, skewness $-1 \leq \beta \leq 1$
- ∞ variance except NORMAL RV $\alpha = 2$
- characteristic function $\langle e^{ikS(\alpha,\beta)} \rangle = e^{-\varphi_{\alpha,\beta}(k)}$
- $\varphi_{\alpha,\beta}(k) = |k|^{\alpha}(1 - i\beta \mathrm{sign}(k) \tan \frac{\pi\alpha}{2})$, $\varphi_{\alpha,-\beta}(k) = \varphi_{\alpha,\beta}(-k)$

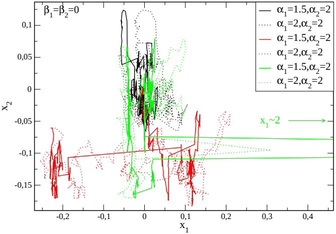
4.3. The word "stable"

- stable w.r.t what? for random variables
- the distribution of the sum of independent identically distributed variables
- $\mathcal{S}_1$ and $\mathcal{S}_2$ independent, distributed as $S(\alpha, \beta) \Rightarrow$ $\mathcal{S}_1 + \mathcal{S}_2 \overset{d}{=} 2^{1/\alpha} S(\alpha, \beta)$
- $\mathcal{S}_1, ..., \mathcal{S}_n$ independent, distributed as $S(\alpha, \beta) \Rightarrow$ $\mathcal{S}_1 + ... + \mathcal{S}_n \overset{d}{=} n^{1/\alpha} S(\alpha, \beta)$
- consequence: $dL_{\alpha,\beta}([t, t + dt[) \overset{d}{=} -dt^{1/\alpha} \cos \frac{\pi\alpha}{2} S(\alpha,\ \beta)$ can hold for all dt, and $L_{\alpha,\beta}(t) \overset{d}{=} -t^{1/\alpha} \cos \frac{\pi\alpha}{2} S(\alpha,\ \beta)$

4.4. Stable variables are attractors

- why studying stable random variables?
- because they are attractors
- Gaussian variables are attractors: Y_i independent copies of Y whose variance is finite, there exist a_n and b_n s.t $\sum a_i Y_i - b_i \Rightarrow G$
- if Y_i independent, distributed as Y whose p.d.f falls of as $x^{-\alpha-1}$ at ∞: $\sum a_i Y_i - b_i \Rightarrow S(\alpha, \beta)$
- ubiquitous in Nature

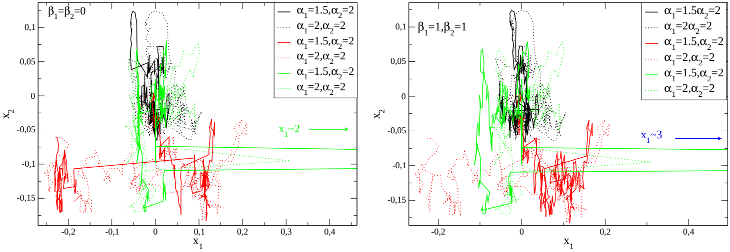
4.5. Stable Lévy motion in 1D and 2D



- $dX([t, t+dt[) = u(X(t)dt + D^{1/\alpha} dL_{\alpha,\beta}([t, t+dt[)$ and $X(0)$: process of p.d.f C solution of $\partial_t C = \partial_x[-uC] + D[p\frac{\partial^\alpha C}{\partial_+ x^\alpha} + (1-p)\frac{\partial^\alpha C}{\partial_- x^\alpha}]$ with $\beta = 2p - 1$
- $d\mathbf{L}_{\alpha_1,\alpha_2,\beta_1,\beta_2}([t, t+dt[)$ independent of the past
- $d\mathbf{L}_{\alpha_1,\alpha_2,\beta_1,\beta_2}([t, t+dt[) \overset{d}{=} -\begin{pmatrix} dt^{1/\alpha_1} \cos\frac{\pi\alpha_1}{2} & 0 \\ 0 & dt^{1/\alpha_2} \cos\frac{\pi\alpha_2}{2} \end{pmatrix}$

- $\frac{\partial C}{\partial t}(\mathbf{x},\ t) + \boldsymbol{\nabla}\cdot\mathbf{u}(\mathbf{x},\ t)C(\mathbf{x},\ t) = \boldsymbol{\nabla}\cdot\overline{\overline{\mathbf{D}}}\nabla_{\boldsymbol{p}}^{\boldsymbol{\alpha}-\mathbf{1}}C(\mathbf{x},\ t) + S_c(\mathbf{x},\ t)$
- $\nabla_{\boldsymbol{p}}^{\boldsymbol{\alpha}-\mathbf{1}}C \equiv \begin{pmatrix} p_1\frac{\partial^{\alpha_1-1}C}{\partial_+ x_1^{\alpha_1-1}} + (1-p_1)\frac{\partial^{\alpha_1-1}C}{\partial_- x_1^{\alpha_1-1}} \\ p_2\frac{\partial^{\alpha_2-1}C}{\partial_+ x_2^{\alpha_2-1}} + (1-p_2)\frac{\partial^{\alpha_2-1}C}{\partial_- x_2^{\alpha_2-1}} \end{pmatrix}$

4.6. Skewness parameter and trajectories



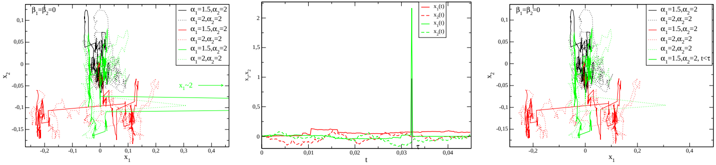
5. Stable Lévy motion density and space fractional diffusion

5.1. In R^2

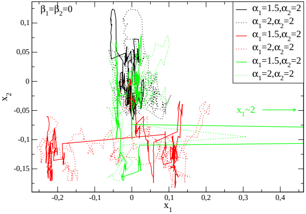
- $d\mathbf{X}([t, t+dt[) =$
  $$\mathbf{u}(\mathbf{X}(t))dt + D^{1/\alpha} \begin{pmatrix} D_1^{1/\alpha_1} & 0 \\ 0 & D_2^{1/\alpha_2} \end{pmatrix} d\mathbf{L}_{\boldsymbol{\alpha},\boldsymbol{\beta}}([t, t+dt[)$$
- $\mathbf{X}(0)$ random variable of $\mathbb{R}^2$, $\boldsymbol{\beta} = 2\mathbf{p} - \mathbf{1}$
- $\frac{\partial C}{\partial t}(\mathbf{x},\ t) + \boldsymbol{\nabla} \cdot \mathbf{u}(\mathbf{x},\ t)C(\mathbf{x},\ t) = \boldsymbol{\nabla} \cdot \overline{\overline{\mathbf{D}}} \nabla_{\boldsymbol{p}}^{\boldsymbol{\alpha}-\mathbf{1}} C(\mathbf{x},\ t) + S_c(\mathbf{x},\ t)$
- $\nabla_{\boldsymbol{p}}^{\boldsymbol{\alpha}-\mathbf{1}} C \equiv \begin{pmatrix} p_1 \frac{\partial^{\alpha_1 - 1} C}{\partial_+ x_1^{\alpha_1 - 1}} + (1 - p_1) \frac{\partial^{\alpha_1 - 1} C}{\partial_- x_1^{\alpha_1 - 1}} \\ p_2 \frac{\partial^{\alpha_2 - 1} C}{\partial_+ x_2^{\alpha_2 - 1}} + (1 - p_2) \frac{\partial^{\alpha_2 - 1} C}{\partial_- x_2^{\alpha_2 - 1}} \end{pmatrix}$

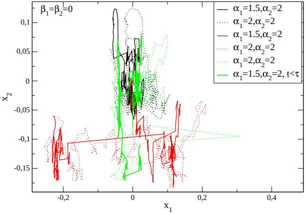
5.2. In bounded domain Ω, $C = 0$ on $\partial\Omega$

Killing $\mathbf{X}(t)$ at 1st exit time τ from Ω yields $\mathbf{X}^{\Omega}(t)$ [Chen, Meerschaert, Nane (2012)] .



5.2. Killing $\mathbf{X}(t)$ at 1st exit time τ from Ω





$$\Omega = [-1,1] \times [-1,1]$$

5.2. In bounded domain Ω, $C = 0$ on $\partial\Omega$

The density of $\mathbf{X}^{\Omega}(t)$ satisfies
$\frac{\partial C}{\partial t}(\mathbf{x},\ t) + \boldsymbol{\nabla} \cdot \mathbf{u}(\mathbf{x},\ t)C(\mathbf{x},\ t) = \boldsymbol{\nabla} \cdot \overline{\overline{\mathbf{D}}}\nabla_{\boldsymbol{p}}^{\boldsymbol{\alpha}-\mathbf{1}} C(\mathbf{x},\ t) + S_c(\mathbf{x},\ t)$ and
$C = 0$ on $\partial\Omega$

Conclusion

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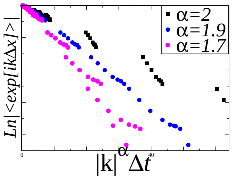

- 2 approaches of super-dispersion. why?
- numerical simulation: the equivalence validates codes
- experiments: sometimes we measure tracer concentrations, sometimes we measure other functionals related to the statistics of molecular motion.

- Example: the characteristic function of water molecule displacement $\langle e^{ik\Delta x}\rangle$. If stable motion rules molecular motion, $= e^{iku\Delta t - D\Delta t\varphi}$, $\varphi = |k|^{\alpha}(1 - i\beta \mathrm{sign}(k) \tan\frac{\pi\alpha}{2})$

Conclusion

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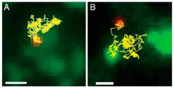
Strange behaviour – albatrosses fly by the rules of anomalous diffusion



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- sometimes we measure individual trajectories, and some mathematical properties attached to parameter α help us discriminating betwen models