Probabilistic Interpretation of Nonlocal Diffusion

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Outline

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Overview

We give a probabilistic interpretation of the nonlocal diffusion equation,

$$u_t(x,t) = \frac{1}{\lambda} \int_{\mathbb{R}} \big(u(y,t) - u(x,t)\big)\phi(x-y)\, \mathrm{d}y,$$

as the master equation for a Markovian CTRW.

We discuss volume constraints, which play the role of boundary conditions on the nonlocal diffusion equation, and describe the inherited constraints on the CTRWs.

We generalize nonlocal diffusion to include temporal effects and thus gain the capability of studying non-Markovian CTRWs.

We investigate more complicated stochastic processes, via the Lévy-Khintchine decomposition, and relationships to the mathematical analysis in (Du and Zhou, 2010) and nonlocal advection (Lehoucq, Kamm, and Parks, 2011).

Probabilistic Interpretation of Diffusion Equations

The classical diffusion equation, a model for classical diffusion,

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sketch of proof: the characteristic function of X_t is given by

$$\varphi_{X_t}(\xi) = \mathbb{E}(e^{i\xi X_t}) = \widehat{u}(\xi,t) = \cdots = \exp(-|\xi|^2 t).$$

Then, note that $\varphi_{X_t}(\xi)$ solves

$$\widehat{u}_t(\xi,t) = -|\xi|^2\widehat{u}(\xi,t).$$

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The nonlocal diffusion equation, a model for anomalous diffusion,

$$u_t(x,t) = \frac{1}{\lambda}\int_{\mathbb{R}} \big(u(y,t) - u(x,t)\big)\phi(x-y)\,\mathrm{d}y,$$

is the master equation for $X_t = \sum_{k=1}^{N_t} R_k$

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Markovian CTRWs on Bounded Domains

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The resulting equations are the master equations for CTRWs on bounded domains with inherited boundary conditions.

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Non-Markovian CTRWs on Bounded Domains

The equation

$$u_t(x,t) = \int_0^t \Lambda(t-t') \int_{\mathbb{R}} \Big(u(y,t')J(y,x) - u(x,t')J(x,y) \Big)\, \mathrm{d}y\, \mathrm{d}t'.$$

is the master equation for an arbitrary CTRW.

The memory kernel Λ is capable of incorporating

- temporal memory effects in the diffusion process
- non-Markovian effects in the CTRW

Augmenting with volume constraints gives us the capability of studying non-Markovian CTRWs on bounded domains via master equations.

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1. "nonlocal", in contrast to $u_t(x,t) = u_{xx}(x,t)$
2. u is a probability density
3. $\lambda > 0$ and has units of time (mean wait-time)
4. ϕ is a symmetric probability density function (in $L^1(\mathbb{R})$)

   hint: ϕ is a propagator function or dispersal kernel, i.e.,

   $$\phi(x-y) = \phi(y-x)$$

   represents the mechanism for stepping from x to y

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(a) a model for anomalous diffusion processes in which the diffusing particle satisfies

$$\langle X^2(t)\rangle \sim t^{\gamma}, \quad \gamma \neq 1$$

note: such processes have been observed experimentally:

- contaminant flow in groundwater
- sporadic movement of foraging spider monkeys
- dynamic motions in proteins
- turbulence in fluids
- dynamics of financial markets
- long-range population/disease dispersion

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(b) an alternative to classical diffusion when Fick's first law is not a valid constitutive relation

note: this equation arises from the classical balance law

$$u_t(x,t) = -q_x(x,t)$$

and a nonlocal flux (Noll, 1955)

$$q(x,t) = -\frac{1}{2}\frac{1}{\lambda}\int_{\mathbb{R}}\int_0^1 \big(u(x+(1-\mu)z,t) - u(x-\mu z,t)\big)z\phi(z)\,\mathrm{d}\mu\,\mathrm{d}z$$

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(c) as the master equation for a compound Poisson process,

$$X_t = \sum_{k=1}^{N_t} R_k$$

1. N_t is a Poisson process with intensity $1/\lambda$
2. $R_k \overset{iid}{\sim} \phi$ and independent of N_t

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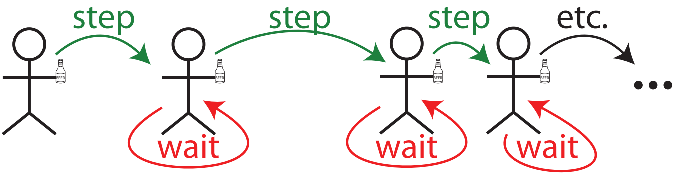

Figure: Illustration of the drunkard's walk.

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sketch of proof: $\varphi_{X_t}(\xi)$ is given by (Lévy-Khintchine)

$$\varphi_{X_t}(\xi) = \exp\left(\frac{1}{\lambda}(\widehat{\phi}(\xi) - 1)t\right)$$

and solves

$$\widehat{u}_t(\xi,t) = \frac{1}{\lambda}(\widehat{\phi}(\xi) - 1)\widehat{u}(\xi,t)$$

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(d) suppose $\widehat{\phi}(\xi) = 1 - \varepsilon^2|\xi|^2 + \text{h.o.t.}$ and $\lambda = \varepsilon^2$, then there is a relationship to fractional diffusion as $\varepsilon \to 0$:

$$\widehat{u}_t(\xi,t) = \frac{1}{\varepsilon^2}(\widehat{\phi} - 1)\widehat{u}(\xi,t) \approx -|\xi|^2\widehat{u}(\xi,t),$$

which is the Fourier transform of the classical diffusion equation

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and, thus, the Lévy Continuity Theorem gives

$$\sum_{k=1}^{N_t} R_k \xrightarrow{d} \sqrt{2}W_t$$

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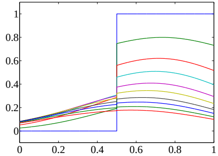
$$\sum_{k=1}^{N_t} R_k \xrightarrow{d} L_t^\alpha$$

Nonlocal Diffusion (in free space)

The effect of α as $\varepsilon \to 0$ for $u_0(x) = \chi_{(1/2,1)}(x)$.



(a) $\varepsilon = 0.2, \alpha = 2$

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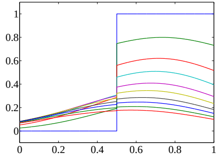
The effect of α as $\varepsilon \to 0$ for $u_0(x) = \chi_{(1/2,1)}(x)$.



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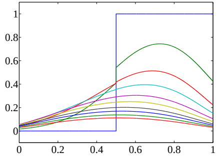
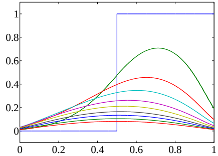
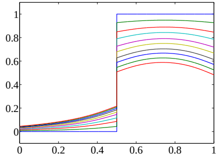


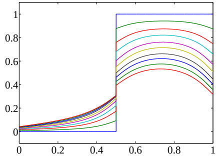
(b) $\varepsilon = 0.1, \alpha = 2$



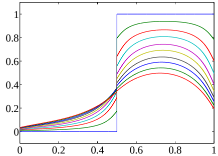
(c) $\varepsilon = 0.05, \alpha = 2$



(d) $\varepsilon = 0.2, \alpha = 1$



(e) $\varepsilon = 0.1, \alpha = 1$



(f) $\varepsilon = 0.05, \alpha = 1$

Figure: We show the solution on $\Omega = (0,1)$ for 10 values of time (pretend $\Omega = \mathbb{R}$).

Outline

1. Overview
2. Master Equations for Markovian CTRWs
   - Nonlocal Diffusion (in free space)
   - Nonlocal Diffusion (on a bounded domain)
3. Other Topics and Ideas
   - Non-Markovian CTRWs
   - Lévy-Khintchine Decomposition
   - Probability and Smoothing
   - Nonlocal Advection (maybe...?)

Nonlocal Diffusion (on a bounded domain)

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$$u_t(x,t) = \frac{1}{\lambda}\int_{\mathbb{R}} \big(u(y,t) - u(x,t)\big)\phi(x-y)\,\mathrm{d}y,$$

on a bounded domain.

1. let Ω denote a bounded domain, for simplicity $\Omega = (0,1)$
2. $u_0(x) \geq 0$ and $\displaystyle\int_{\Omega} u_0(x)\,\mathrm{d}x = 1$
3. we consider two types of boundary conditions:
   a. "Dirichlet" volume constraints, i.e., CTRW with absorbing boundaries
   b. "Neumann" volume constraints, i.e., CTRW with insulated boundaries

"Dirichlet" Constraints / Absorbing Boundaries

Consider the nonlocal "Dirichlet" problem,

$$\begin{cases} u_t(x,t) = \dfrac{1}{\lambda}\displaystyle\int_{\mathbb{R}} \big(u(y,t) - u(x,t)\big)\phi(x-y)\,\mathrm{d}y, & x \in \Omega, \\ u(x,t) = 0, & x \in \mathbb{R}\setminus\Omega, \\ u(x,0) = u_0(x), & x \in \Omega. \end{cases}$$

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In the CTRW framework, this imposes absorbing boundaries.

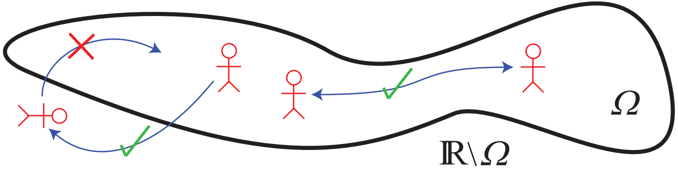

Illustration of absorbing boundaries.

"Neumann" Constraints / Insulated Boundaries

Consider the nonlocal "Neumann" problem,

$$\begin{cases} u_t(x,t) = \dfrac{1}{\lambda}\displaystyle\int_{\Omega} \big(u(y,t) - u(x,t)\big)\phi(x-y)\,\mathrm{d}y, & x \in \Omega, \\ u(x,0) = u_0(x), & x \in \Omega. \end{cases}$$

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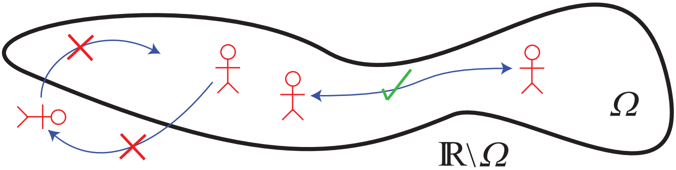

Illustration of insulated boundaries.

Numerical Solutions and Simulations

Conjecture:

(i) the nonlocal “Dirichlet” problem is the master equation for a Markovian CTRW on Ω with absorbing boundaries

(ii) the nonlocal “Neumann” problem is the master equation for a Markovian CTRW on Ω with insulated boundaries

Numerical Solutions and Simulations

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evidence:

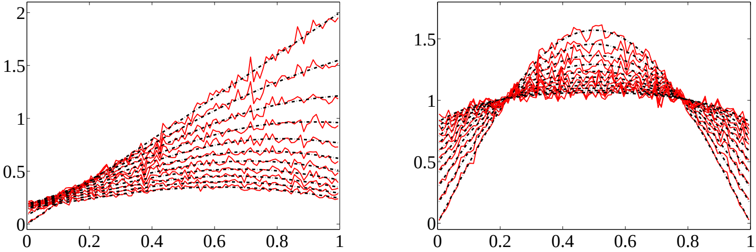
- compute numerical solutions, u_h, via a finite element method
- compute kernel density estimates, μ_N, from N simulations
- show $\|\mu_N - u_h\| \to 0$ as $h \to 0$ and $N \to \infty$

note: $\|\mu_N - u_h\| \leq \underbrace{\|\mu_N - u\|}_{\text{sampling}} + \underbrace{\|u_h - u\|}_{\text{numerical}}$

Numerical Solutions and Simulations

We compare numerical solutions to results from CTRW simulations

- u_h is the numerical solution of the master equation (black)
- μ_N is the kernel density estimate from simulations (red)



(a) $u_0(x) = 2x$ (b) $u_0(x) = \frac{\pi}{2}\sin(\pi x)$

Figure: Left: absorbing boundaries. Right: insulated boundaries.

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Non-Markovian CTRWs

Next consider the master equation for an arbitrary CTRW,

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$$u_t(x,t) = \frac{1}{\lambda} \int_{\mathbb{R}} \big(u(y,t) - u(x,t)\big)\phi(x-y)\, \mathrm{d}y,$$

is a special (Markovian) case that arises when $\Lambda(t-t') = \frac{1}{\lambda}\delta(t-t')$ and $J(x,y) = J(y,x) = \phi(x-y)$

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The memory kernel Λ is capable of incorporating temporal, e.g., non-Markovian, effects and is related to the wait-time density ω via

$$\widehat{\Lambda}(s) = \frac{s\widehat{\omega}(s)}{1-\widehat{\omega}(s)}.$$

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Taking $\Lambda(t-t') = \frac{1}{\tau^2} \exp\left(-\frac{t-t'}{\tau/2}\right)$, i.e., $\omega \sim$ Gamma$(2,\tau)$, we arrive at the nonlocal Cattaneo-Vernotte equation

$$u_t(x,t) + \frac{\tau}{2} u_{tt}(x,t) = \frac{1}{2\tau} \int_{\mathbb{R}} \big(u(y,t) - u(x,t)\big) \phi(x-y) \, \mathrm{d}y.$$

Non-Markovian CTRWs

The nonlocal Cattaneo-Vernotte equation,

$$u_t(x,t) + \frac{\tau}{2} u_{tt}(x,t) = \frac{1}{2\tau} \int_{\mathbb{R}} \big(u(y,t) - u(x,t)\big)\phi(x-y)\,\mathrm{d}y,$$

- is the master equation for a renewal-reward process
- is the nonlocal version of the classical Cattaneo-Vernotte equation

$$u_t(x,t) + \frac{\tau}{2} u_{tt}(x,t) = D\Delta u(x,t)$$

remark: (as we did in the Markovian case) we can study non-Markovian CTRWs on bounded domains via the associated master equation

Outline

Lévy-Khintchine Decomposition

Definition: Infinitely Divisible Distribution

A distribution F of a random variable X is infinitely divisible if, for any $n \in \mathbb{N}$, there exists $X_i \overset{iid}{\sim} G$ such that

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The Lévy-Khintchine decomposition characterizes all infinitely divisible processes.

Lévy-Khintchine Decomposition

Definition: Infinitely Divisible Distribution

A distribution F of a random variable X is infinitely divisible if, for any $n \in \mathbb{N}$, there exists $X_i \overset{iid}{\sim} G$ such that

$$\sum_{i=1}^{n} X_i \overset{d}{=} X .$$

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The Lévy-Khintchine decomposition thus characterizes all Lévy processes.

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Let $b \in \mathbb{R}$, $c \in \mathbb{R}_{\geq 0}$, and ϕ (relaxing earlier assumptions) be such that

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Then, there is a Lévy process L_t consisting of four independent processes (drift, diffusion, compound Poisson, square-integrable martingale) such that

$$\varphi_{L_t}(\xi) = \exp\left(t\left(i\xi b - \frac{\xi^2 c}{2} + \int_{|x|\geq\delta}\left(e^{i\xi x} - 1\right)\phi(x)\,\mathrm{d}x + \int_{|x|<\delta}\left(e^{i\xi x} - 1\right)\phi(x)\,\mathrm{d}x\right)\right).$$

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A little work demonstrates the master equation is

$$u_t(x,t) = b\frac{\partial u}{\partial x}(x,t) + \frac{c}{2}\frac{\partial^2 u}{\partial x^2}(x,t) + \int_{\mathbb{R}} \big(u(y,t) - u(x,t)\big)\phi(x-y)\, \mathrm{d}y.$$

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If we ignore drift and diffusion...

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Let $b = 0$, $c = 0$, and ϕ be such that

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(a) $\int_{\mathbb{R}} \phi(x)\,\mathrm{d}x < \infty$, a.s. a finite number of steps on every compact interval, finite activity

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One can show that u is the density of a Lévy $2s$-stable process, i.e.,

$$u_t(x,t) = -(-\Delta)^s u(x,t).$$

Outline

Relationship to (Du and Zhou, 2010)

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observation: “activity” of process = “smoothing” of operator

Outline

1. Overview
2. Master Equations for Markovian CTRWs
   - Nonlocal Diffusion (in free space)
   - Nonlocal Diffusion (on a bounded domain)
3. Other Topics and Ideas
   - Non-Markovian CTRWs
   - Lévy-Khintchine Decomposition
   - Probability and Smoothing
   - Nonlocal Advection (maybe...?)

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Let ϕ be such that

$$\boxed{\int_{\mathbb{R}} x\phi(x)\,\mathrm{d}x = \mu < \infty} \qquad \text{and} \qquad \int_{\mathbb{R}} (1 \wedge |x|^2)\phi(x)\,\mathrm{d}x < \infty.$$

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note: these are both (potentially) biased now

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Consider $\phi_\varepsilon(x-y) = \frac{1}{\varepsilon}\cdot\frac{1}{\varepsilon}\phi\left(\frac{x-y}{\varepsilon}\right)$ so that

$$\begin{aligned} u_t(x,t) &= \int_{\mathbb{R}} \big(u(y,t) - u(x,t)\big)\phi_\varepsilon(x-y)\,\mathrm{d}y \\ &= \int_{\mathbb{R}} \left((y-x)\frac{\partial u}{\partial x}(x,t) + \frac{(y-x)^2}{2}\frac{\partial^2 u}{\partial x^2}(x,t) - \cdots\right)\phi_\varepsilon(x-y)\,\mathrm{d}y \\ &= -\mu\frac{\partial u}{\partial x}(x,t) + O(\varepsilon). \end{aligned}$$

Thanks! and Questions?

I'd like to thank

- Dr. Richard Lehoucq and Sandia National Laboratories
- Dr. Don Estep and Colorado State University
- the organizers of this mini-workshop and the MFO
- all of you – it has been a very enjoyable week

I welcome any questions and comments.

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