The exit-time problem for a Markov jump process

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Exit-time for Brownian motion

- Define the exit-time random variable

$$T_x := \inf\{t : X_t \in \partial\Omega_d \subseteq \partial\Omega \,\&\, X_0 = x \in \Omega\}$$

  for the diffusion starting at $x \in \Omega$
- The density of particles that have not yet exited Ω to $\partial\Omega_d \subseteq \partial\Omega$

$$\begin{cases} u_t = b \cdot \nabla u + 2D\Delta u & \text{on } \Omega \\ u = 0 & \text{on } \partial\Omega_d \\ u(x,0) = \delta(x) & \text{on } \Omega \end{cases}$$

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Mean exit-time

- Given the solution of the u of the diffusion equation, the mean exit-time is given by

$$\mathbb{E}(T_x) = \int_0^\infty u(x,t)\,dt$$

- We can also determine this mean as the solution of the steady-state problem

$$\begin{cases} \big(b\cdot\nabla + 2D\Delta\big)\mathbb{E}(T_x) = -1 & \text{on } \Omega \\ u = 0 & \text{on } \partial\Omega_d \end{cases}$$

- Repeated integration of the steady-state problem determines all the moments

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Comments

These are classical results; the exit-time problem assumes

- backward Kolmogorov equation (the adjoint of the Fokker-Planck equation)
- diffusion hits the boundary upon exiting Ω
- the mean (and other moments) are finite

Markov jump process

Consider the class of Markov jump processes, described by the master equation

$$u_t(x,t) = \int_{\mathbb{R}^n} \gamma(y,x)\, u(y,t)\, dy - \int_{\mathbb{R}^n} \gamma(x,y)\, u(x,t)\, dy$$

The process...

- can be approximated as a continuous-time Markov chain, or an off-lattice CTRW with an exponential jump-rate,
- is spatially inhomogeneous when the jump-rate is not invariant under translations

Finite range Markov jump process

What if we want to consider

- the exit-time problem and link with a deterministic equation?
- jump at most a finite distance away?

My presentation explains how to do exactly this, that the problem is well-posed and that high-quality discretizations are available

Finite range jump processes

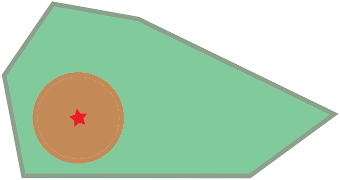
- Jump-rate $\gamma(x, y)$ is of compact support for each x; particle can jump at most a finite distance away, e.g., let ν be an asymmetric finite Lévy measure

$$\gamma(x, y) = \mathbb{1}_\Omega(x)\mathbb{1}_\Omega(y)\nu(x - y)$$

  is spatially inhomogenous
- Such a Markov jump process has no "heavy tails"
- Then $\mathbb{E}\, X_t^2 \propto t$, i.e., finite mean, MSD
- Fluctuations can take on various forms; discontinuous sample path (of the particle) can be of three types
- "Nonlocal convection" associated with asymmetric rate $\gamma(x, y) \neq \gamma(y, x)$

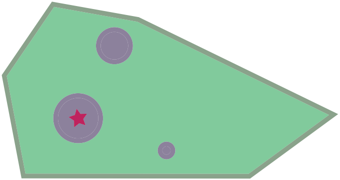
Diffusion applications

- transport in heterogeneous media, heat conduction
- disease transmission, foraging or migrating animals



Brownian motion may not be appropriate due to

- Heterogeneity of the underlying medium
- Nonlocal dispersion, transmission mechanisms



Exit-time via the master equation

- Define the exit-time random variable

$$T_x := \inf\{t : X_t \in \Omega_d \subseteq \Omega_{\mathcal{I}} \,\&\, X_0 = x \in \Omega\}$$

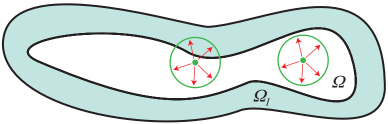
  for the diffusion starting at $x \in \Omega$

- The density of particles that have not yet exited Ω to $\Omega_d \subseteq \Omega_{\mathcal{I}}$

$$\begin{cases} u_t(x,t) = \displaystyle\int_{\Omega \cup \Omega_d} \big(u(y,t)\gamma(y,x) - u(x,t)\gamma(x,y)\big)\, dy & x \in \Omega \\ u(x,t) = 0 \qquad x \in \Omega_d \\ u(x,0) = \delta(x) \qquad x \in \Omega \end{cases}$$

Formulation of volume-constrained problems

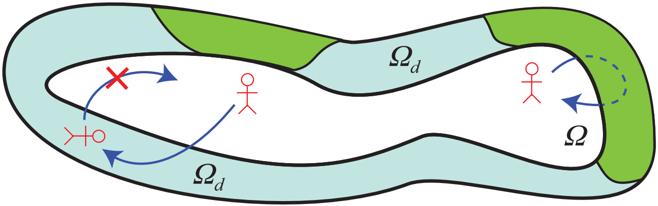
$$u_t(x,t) = \int_{\Omega \cup \Omega_{\mathcal{I}}} \big(u(y,t)\gamma(y,x) - u(x,t)\gamma(x,y)\big)\, dy \qquad x \in \Omega$$



- Constraints on u over the volume $\Omega_{\mathcal{I}} \subseteq \mathbb{R}^n \setminus \Omega$—boundary conditions are NOT well-defined because sample path, with probability 1, jumps out of Ω into $\Omega_{\mathcal{I}}$ (Millar 1975)
- $\Omega_{\mathcal{I}}$ is the "interaction region"
- A link with a deterministic equation can be established

Absorbed/censored process

$\emptyset \neq \Omega_d \subsetneq \Omega_{\mathcal{I}}$ is a mixed process with a mixed volume constraint; nonlocal analogue of a mixed Dirichlet, Neumann boundary value problem



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Mean exit-time cases

$\Omega_d \equiv \Omega_{\mathcal{I}}$

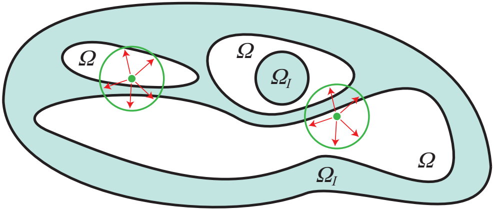
- Absorbed process with a homogenous Dirichlet volume constraint problem
- Probability is conserved over $\Omega \cup \Omega_d$, i.e., the process is either in Ω or has exited to Ω_d

$\Omega_d \equiv \emptyset$

- Censored process with a pure Neumann volume constraint problem; particle confined to a box
- Probability is conserved over Ω, i.e., the process remains in Ω

Escape probabilities

- Volume-constrained problems allow for “non-standard” domains, e.g., unconnected domains



- Decomposition into escape probabilities

$$\int_{\Omega} u(x,t)\,dx = 1 - \sum_k \sum_j M_{\Omega_j}^{\Omega_{\mathcal{I}_k}}(t)$$

Mathematical Analysis

- Goal: show that the nonlocal diffusion equation for the exit-time problem is well-posed
- Introduce a nonlocal vector calculus, an alternative to fractional derivatives—forward and backward Kolmogorov equations are then easily determined
- Show that the steady-state equation is well-posed
- Then, standard results demonstrate that the nonlocal diffusion equation is well-posed
- Stable, robust numerical methods offer an alternative to Monte-Carlo simulation

Steady-state nonlocal diffusion

$$\begin{cases} -\mathcal{L}u = b & \text{on } \Omega \subseteq \mathbb{R}^n \\ u = 0 & \text{on } \Omega_{\mathcal{I}} \subseteq \mathbb{R}^n \setminus \Omega, \end{cases}$$

where

$$\mathcal{L}\, u(x) = \int_{\Omega \cup \Omega_{\mathcal{I}}} \big(u(y,t)\gamma(y,x) - u(x,t)\gamma(x,y)\big)\, dy$$

$$\Omega_{\mathcal{I}} = \Omega_d$$

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Nonlocal divergence

- Let $\boldsymbol{\alpha}, \mathbf{f} : \mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{R}^3, \boldsymbol{\alpha}(x, y) = -\boldsymbol{\alpha}(y, x)$

$$\mathcal{D}(\mathbf{f})(x) := \int_{\mathbb{R}^3} \big(\mathbf{f}(x, y) + \mathbf{f}(y, x)\big) \cdot \boldsymbol{\alpha}(x, y)\, dy$$

  where $\mathcal{D}(\mathbf{f}) : \mathbb{R}^3 \to \mathbb{R}$
- Only the symmetric part of **f** matters
- $\mathcal{D}$ is a distributional divergence because

$$\boldsymbol{\alpha}(x, y) = -\frac{\partial}{\partial y}\delta(y - x) \Longrightarrow \mathcal{D}(\mathbf{f})(x) \equiv \nabla \cdot \mathbf{f}(x, x)$$

Adjoint operator

- Recall that $\alpha(x, y) = -\alpha(y, x)$ and define

$$\mathcal{D}^*(u)(x, y) := -\big(u(y) - u(x)\big)\,\alpha(x, y)$$

where $\mathcal{D}^* u : \mathbb{R} \to \mathbb{R}^3$

- $\mathcal{D}^*$ is a distributional gradient because

$$\alpha(x, y) = -\frac{\partial}{\partial y}\delta(y - x) \Longrightarrow \int_{\mathbb{R}^3} \mathcal{D}^* u \, dy = -\nabla u$$

- Can show $\mathcal{D}^*$ is the adjoint to $\mathcal{D}$ via a nonlocal Green's first identity

Steady-state nonlocal diffusion via the nonlocal calculus

$$\begin{cases} -\mathcal{L}\, u = b & \text{on } \Omega \subseteq \mathbb{R}^n \\ \quad u = 0 & \text{on } \Omega_{\mathcal{I}} \subseteq \mathbb{R}^n \setminus \Omega\,, \end{cases}$$

or

$$\begin{cases} \mathcal{D} \cdot \mathbf{f} = b & \text{on } \Omega \subseteq \mathbb{R}^n \\ \quad \mathbf{f} = \boldsymbol{\mu}\, u + \boldsymbol{\Theta}\, \mathcal{D}^* u & \\ \quad u = 0 & \text{on } \Omega_{\mathcal{I}} \subseteq \mathbb{R}^n \setminus \Omega\,, \end{cases}$$

where

$$\begin{aligned} \mathcal{L}\, u &= \int_{\Omega \cup \Omega_{\mathcal{I}}} \big(u(y,t)\gamma(y,x) - u(x,t)\gamma(x,y) \big)\, dy \\ &= \mathcal{D}\big(\mathcal{D}^* u\big)(x) + \mathcal{D}\big(\boldsymbol{\mu} u\big)(x) \\ \gamma(x,y) &= \boldsymbol{\alpha}(x,y) \cdot \big(\boldsymbol{\Theta}(x,y)\boldsymbol{\alpha}(x,y) \big) - \boldsymbol{\mu}(x,y) \cdot \boldsymbol{\alpha}(x,y) \end{aligned} \tag{1}$$

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Nonlocal divergence theorem

- The definition of the nonlocal divergence grants

$$\int_{\Omega} \mathcal{D}(\mathbf{f})\, dx = -\int_{\Omega_{\mathcal{I}}} \mathcal{D}(\mathbf{f})\, dx$$

- Immediate consequence is the well-formulated conservation law

$$\frac{d}{dt}\int_{\Omega} u\, dx = -\int_{\Omega} \mathcal{L}\, u\, dx = \underbrace{\int_{\Omega_{\mathcal{I}}} \mathcal{D}(\mathcal{D}^{*} u - \mu\, u)\, dx}_{\text{probability flux out of } \Omega \text{ into } \Omega_{\mathcal{I}}}$$

- A well defined notion of a flux is equivalent to the antisymmetry in x, y of the integrand, and action-reaction, and lack of self-interaction

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Nonlocal integration by parts

- *Nonlocal* Green's first identity

$$\int_{\Omega} v\mathcal{D}(\mathcal{D}^* u)\, dx - \int_{\Omega\cup\Omega_{\mathcal{I}}} \int_{\Omega\cup\Omega_{\mathcal{I}}} \mathcal{D}^* v \cdot \mathcal{D}^* u\, dy\, dx$$
$$= - \int_{\Omega_{\mathcal{I}}} v\, \mathcal{D}(\mathcal{D}^* u)\, dx$$

Compare with the classical version

$$\int_{\Omega} v \Delta u\, dx + \int_{\Omega} \nabla v \cdot \nabla u\, dx = \int_{\partial\Omega} v \left(\nabla u \cdot \mathbf{n}\right) ds$$

- Can show that

$$\int_{\Omega_{\mathcal{I}}} v\, \mathcal{D}(\mathcal{D}^* u)\, dx = \int_{\partial\Omega} v\, \left(\mathcal{D}^* u \cdot \mathbf{n}\right) dS \qquad \forall v \in C_0^{\infty}$$

Nonlocal variational problem

- Find $u \in V$ such that

$$a(u,v) = \int_{\Omega} u\, b\, dx \qquad \forall\, v \in V$$

where

$$a(u,v) = \int_{\Omega\cup\Omega_{\mathcal{I}}} \int_{\Omega\cup\Omega_{\mathcal{I}}} \mathcal{D}^* u \cdot \mathbf{\Theta}\, \mathcal{D}^* v\, dy\, dx - \int_{\Omega} \mathcal{D}\big(\boldsymbol{\mu} u\big)\, v\, dx$$

- Lax-Milgram theorem implies that the Euler-Lagrange equations are well-posed, the energy is bounded by the data

$$\int_{\Omega\cup\Omega_{\mathcal{I}}} \int_{\Omega\cup\Omega_{\mathcal{I}}} |\mathcal{D}^* u|^2\, dy\, dx \le C \int_{\Omega} b^2\, dx$$

Comments

- Can identify space V with square integrable functions or a fractional Sobolev space given conditions on the integrability of the jump-rate γ
- In particular, for infinite activity and finite variation sample path $\iff \int |y| \, \gamma(x, y) \, dy < \infty$, we have a first of a kind result
- If $\gamma(x, y) = \gamma(y, x)$ then the variational problem is the Euler-Lagrange equation for

$$\min_V \frac{1}{2} a(u, v) - \int_\Omega u \, b \, dx$$

- Volume constraint is crucial for the mathematical analysis and link with the Markov jump process; boundary conditions may not be meaningful

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