Fractional Diffusion Equations

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Overview

Stochastic Model

Random Walk in 1D

- at time $t = 0$, random walker is in position $x = 0$
- random walker jumps at times $t = n\tau$ $(n = 1, 2, \ldots)$
  where $\tau > 0$ is a fixed constant
- jump length $= \xi > 0$ (the lattice constant; also fixed)
- direction of jump is randomly chosen;
  equal probabilities for jumps to right and to left
- Notation: $P(x, t) \cdot \xi =$ probability that random walker's position
  at time t is in interval $[x, x + \xi)$
- master equation:

$$P(x, t + \tau) = \frac{1}{2} P(x + \xi, t) + \frac{1}{2} P(x - \xi, t)$$

Stochastic Model

Master equation:

$$P(x, t+\tau) = \frac{1}{2} P(x+\xi, t) + \frac{1}{2} P(x-\xi, t)$$

Taylor expansion:

$$P(x, t+\tau) = P(x, t) + \tau \frac{\partial P}{\partial t}(x, t) + O\left(\tau^2\right)$$

$$P(x \pm \xi, t) = P(x, t) \pm \xi \frac{\partial P}{\partial x}(x, t) + \frac{\xi^2}{2} \frac{\partial^2 P}{\partial x^2}(x, t) + O\left(\xi^3\right)$$

Plug into master equation and rearrange:

$$\frac{\partial P}{\partial t}(x, t) = \frac{\xi^2}{2\tau} \frac{\partial^2 P}{\partial x^2}(x, t) + \xi \cdot O\left(\frac{\xi^2}{\tau}\right) + O(\tau)$$

Continuum Limit

$$\frac{\partial P}{\partial t}(x,t) = \frac{\xi^2}{2\tau}\frac{\partial^2 P}{\partial x^2}(x,t) + \xi \cdot O\left(\frac{\xi^2}{\tau}\right) + O(\tau)$$

Continuum limit ($\tau \to 0$ and $\xi \to 0$ coupled such that diffusion coefficient $d_1 = \lim_{\tau\to 0, \xi\to 0} \xi^2/(2\tau)$ exists):

$$\frac{\partial P}{\partial t}(x,t) = d_1 \frac{\partial^2 P}{\partial x^2}(x,t) \qquad \text{(classical diffusion equation)}$$

Can be generalized to n-dimensional case:

$$\frac{\partial P}{\partial t}(x,t) = d_1 \Delta P(x,t) \qquad \text{where} \quad \Delta = \sum_{j=1}^{n} \frac{\partial^2}{\partial x_j^2} \quad \text{(Laplace operator)}$$

Solution of Classical Diffusion Equation

- Diffusion equation:

$$\frac{\partial P}{\partial t}(x,t) = d_1 \frac{\partial^2 P}{\partial x^2}(x,t)$$

- Random walker located in position $x = 0$ at time $t = 0$
  $\Rightarrow$ initial condition $P(x,0) = \delta(x)$ (Dirac distribution)
- Solution of initial value problem:

$$P(x,t) = \frac{1}{\sqrt{4\pi d_1 t}} \exp\left(-\frac{x^2}{4 d_1 t}\right)$$

- For fixed t, $P(\cdot, t)$ is (spatial) Gaussian distribution with mean value $\mu = 0$ and standard deviation $\sigma(t) = \sqrt{2 d_1 t}$
  $\Rightarrow$ mean squared displacement of random walker at time t is

$$\sigma^2(t) = 2 d_1 t$$

Outlook

Classification of diffusion processes according to behaviour of mean squared displacement at time t (when t is large):

$$\sigma^2(t) \sim t^{\alpha} \qquad \text{for } t \to \infty$$

- classical diffusion (see above): $\alpha = 1$
- subdiffusion: $\alpha < 1$
- superdiffusion: $\alpha > 1$
- ballistic diffusion: $\alpha = 2$

Next steps:
Find mathematical models that exhibit such kinds of behaviour

Limitations of Stochastic Model

Random Walk in 1D

- at time $t = 0$, random walker is in position $x = 0$
- random walker jumps at times $t = n\tau$ $(n = 1, 2, \ldots)$ where $\tau > 0$ is a fixed constant
- jump length $= \xi > 0$ (the lattice constant, also fixed)
- direction of jump is randomly chosen; equal probabilities for jumps to right and to left

Many deterministic assumptions!

Continuous-Time Random Walks

- at time $t = 0$, random walker is in position $x = 0$
- joint probability distribution function $\psi(x, t)$ (so-called jump PDF) governs lengths of jumps and waiting time between successive jumps
- jump length PDF:
$$\lambda(x) = \int_0^\infty \psi(x, t)\,\mathrm{d}t$$
- waiting time PDF:
$$w(t) = \int_{-\infty}^\infty \psi(x, t)\,\mathrm{d}x$$
- main characteristic features of CTRW model:
  - characteristic waiting time $T = \int_0^\infty t w(t)\,\mathrm{d}t$ (first moment of w)
  - jump length variance $\Sigma^2 = \int_{-\infty}^\infty x^2 \lambda(x)\,\mathrm{d}x$

Continuous-Time Random Walks

- characteristic waiting time $T = \int_0^\infty t w(t)\,\mathrm{d}t$
- jump length variance $\Sigma^2 = \int_{-\infty}^{\infty} x^2 \lambda(x)\,\mathrm{d}x$

	$T < \infty$	$T = \infty$
$\Sigma^2 < \infty$	classical diffusion (Brownian motion)	(non-Markovian) subdiffusion (time-fractional PDE)
$\Sigma^2 = \infty$	Markovian Lévy flights (space-fractional PDE)	non-Markovian Lévy flights (space-and-time-fractional PDE)

Simplifying assumption:

- jump lengths and waiting times are independent random variables
- $\psi(x,t) = \lambda(x) w(t)$

Continuous-Time Random Walks

$$\begin{aligned}\eta(x,t) &= \text{PDF of just having arrived in position } x \text{ at time } t\\ &= \int_{-\infty}^{\infty}\int_0^{\infty} \eta(\xi,\tau)\psi(x-\xi,t-\tau)\,\mathrm{d}\tau\mathrm{d}\xi + P_0(x)\delta(t)\\ (P_0 &= \text{initial condition})\end{aligned}$$

Then,

$$\begin{aligned}P(x,t) &= \text{PDF of being in position } x \text{ at time } t\\ &= \int_0^t \eta(x,\tau)\Psi(t-\tau)\,\mathrm{d}\tau\end{aligned}$$

where $\Psi(t) = 1 - \int_0^t w(\tau)\,\mathrm{d}\tau$ (“no jump in time interval $[0,t]$”)

Transforming the PDF

Application of Fourier transform in space and Laplace transform in time to this PDF yields

$$\mathcal{F}\mathcal{L}P(\omega, s) = \frac{1 - \mathcal{L}w(s)}{s} \cdot \frac{\mathcal{F}P_0(\omega)}{1 - \mathcal{F}\mathcal{L}\psi(\omega, s)}$$
$$= \frac{1 - \mathcal{L}w(s)}{s} \cdot \frac{\mathcal{F}P_0(\omega)}{1 - \mathcal{F}\lambda(\omega)\mathcal{L}w(s)} \qquad (*)$$

Anomalous Diffusion

Special case: waiting time PDF with heavy tail

$$w(t) \sim A_\alpha \left(\frac{\tau}{t}\right)^{\alpha+1} \qquad \text{for } t \to \infty$$

- $\alpha \in (0, 1)$
- $\tau > 0$: characteristic time constant
- $A_\alpha > 0$: normalization factor

Properties:

- w is integrable,
  characteristic waiting time (first moment of w): $T = \infty$.
- Tauberian theorem: $\mathcal{L}w(s) \sim 1 - (s\tau)^\alpha$ as $s \to 0$

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Concrete example:

$$\text{waiting time PDF } w(t) = -\frac{\mathrm{d}}{\mathrm{d}t} E_{\alpha,1}(-t^\alpha)$$

$$\text{with Mittag-Leffler function } E_{\alpha,\beta}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + \beta)} \text{ and } 0 < \alpha < 1$$

$$\text{Gaussian jump length PDF } \lambda(x) = \frac{1}{\sqrt{4\pi\sigma^2}} \exp\left(-\frac{x^2}{4\sigma^2}\right)$$

such that $\Sigma^2 = 2\sigma^2 < \infty$

$$\mathcal{L}w(s) = \frac{1}{1 + s^\alpha}, \qquad \mathcal{F}\lambda(\omega) \sim 1 - \sigma^2\omega^2 \quad (\omega \to 0)$$

Anomalous Diffusion

Recalling

$$\mathcal{F}\mathcal{L}P(\omega, s) = \frac{1 - \mathcal{L}w(s)}{s} \cdot \frac{\mathcal{F}P_0(\omega)}{1 - \mathcal{F}\lambda(\omega)\mathcal{L}w(s)} \qquad (*)$$

and plugging in the above statements $\mathcal{L}w(s) = \frac{1}{1+s^\alpha}$ and $\mathcal{F}\lambda(\omega) \sim 1 - \sigma^2\omega^2$, we obtain for $s \to 0$ and $\omega \to 0$ that

$$\mathcal{F}\mathcal{L}P(\omega, s) \sim \frac{\mathcal{F}P_0(\omega)/s}{1 + d_\alpha \omega^2 s^{-\alpha}}$$

with some constant d_α, or

$$(1 + d_\alpha \omega^2 s^{-\alpha})\mathcal{F}\mathcal{L}P(\omega, s) \sim \frac{\mathcal{F}P_0(\omega)}{s}$$

Anomalous Diffusion

Exploiting Fourier and Laplace transforms and their properties, this yields for large t and $|x|$

$$P(x,t) - P_0(x) = d_\alpha J^\alpha_{0,t} P_{xx}(x,t)$$

where $J^\alpha_{0,t}$ is the Riemann-Liouville integral of order α w.r.t. t.

Equivalent formulation: IVP for time-fractional diffusion equation

$$D^\alpha_{*0,t} P(x,t) = d_\alpha \frac{\partial^2 P}{\partial x^2}(x,t), \qquad P(x,0) = P_0(x),$$

where $D^\alpha_{*0,t}$ is the Caputo derivative of order α w.r.t. t.

Laplace transform techniques lead to

$$\text{mean squared displacement} = \sigma^2(t) = \frac{2d_\alpha}{\Gamma(1+\alpha)} t^\alpha$$

General Formulation

$$D^{\alpha}_{*0,t} u(x,t) = -Lu(x,t) + F(x,t), \qquad x \in G \subset \mathbb{R}^n, \quad t \in (0,T) \quad (\square)$$

- $\alpha \in (0,1]$; $D^{\alpha}_{*0,t}$ is the Caputo derivative of order α w.r.t. t
- G is open and bounded domain in $\mathbb{R}^n$
- $Lu(x,t) = -\operatorname{div}(p(x) \operatorname{grad} u(x,t)) + q(x)u(x,t)$
- $p \in C(\bar{G})$, $q \in C(\bar{G})$, $p(x) > 0$ and $q(x) \geq 0$ for $x \in \bar{G}$

$-L$ is elliptic differential operator of order 2,

$$\begin{aligned} -Lu(x,t) &= \sum_{k=1}^{n} \left(p(x) \frac{\partial^2 u}{\partial x_k^2}(x,t) + \frac{\partial p}{\partial x_k}(x) \frac{\partial u}{\partial x_k}(x,t) \right) - q(x)u(x,t) \\ &= p(x)\Delta u(x,t) + (\operatorname{grad} p(x,t), \operatorname{grad} u(x,t)) - q(x)u(x,t) \end{aligned}$$

Problem $(\square)$ reduces to classical parabolic PDE when $\alpha = 1$

Initial and Boundary Conditions

Same conditions as in classical parabolic PDE
(with time derivative of order 1):

$$
\begin{aligned}
u(x,0) &= u_0(x) && \text{for all } x \in \bar{G}, \\
u(x,t) &= v(x,t) && \text{for all } x \in \partial G \text{ and } t \in [0,T]
\end{aligned}
$$

Definition

A function $u : \bar{G} \times [0, T]$ is called a solution to the IBVP above if

- u is continuous in its domain of definition,
- u is twice differentiable with respect to x in G,
- u is once differentiable with respect to $t \in (0, T]$ such that the first time derivative is in $L^1(0, T)$,
- u satisfies the differential equation (☐) and the initial and boundary conditions above.

Uniqueness of Solutions

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General assumptions (can be weakened):

- forcing function: $F \in C(\bar{G} \times [0, T])$
- initial function: $u_0 \in C(\bar{G})$
- boundary function: $v \in C(\partial G \times [0, T])$

Theorem

Under the given assumptions, the time-fractional IBVP above possesses at most one solution.
The solution depends continuously on F, u_0 and v in the following sense: If u_1 and u_2 are solutions to the PDE ($\square$) with forcing, initial and boundary functions F_1, u_{01} and v_1 or F_2, u_{02} and v_2, respectively, then

$$\|u_1 - u_2\|_{L_\infty(\bar{G}\times[0,T])} \leq \max\left\{\|u_{01} - u_{02}\|_{L_\infty(\bar{G})}, \|v_1 - v_2\|_{L_\infty(\partial G\times[0,T])}\right\} + \frac{T^\alpha}{\Gamma(1+\alpha)}\|F_1 - F_2\|_{L_\infty(\bar{G}\times[0,T])}$$

The Maximum Principle

Theorem

Let u be a solution to the IBVP above under the given assumptions and subject to the condition $F(x,t) \le 0$ for all x and t. Then

- *either $u(x,t) \le 0$ for all x and t*
- *or $u(x,t)$ attains its positive maximum on the part $S = (\bar{G} \times \{0\}) \cup (\partial G \times [0,T])$ of the boundary of its domain of definition,*

i.e.

$$u(x,t) \le \max\left\{0, \max_{(\xi,\tau)\in S} u(\xi,\tau)\right\} \qquad \text{for all } x \text{ and } t.$$

Construction of the Solution

Homogeneous PDE and BC, general IC:

$$D^{\alpha}_{*0,t} u(x,t) = -Lu(x,t) \qquad \text{for all } x \in G \text{ and } t \in (0,T),$$

$$u(x,0) = u_0(x) \qquad \text{for all } x \in \bar{G},$$

$$u(x,t) = 0 \qquad \text{for all } x \in \partial G \text{ and } t \in [0,T]$$

ansatz (Fourier): $u(x,t) = X(x)T(t)$

separation of variables: $\dfrac{D^{\alpha}_{*0} T(t)}{T(t)} = -\dfrac{LX(x)}{X(x)} = -\lambda$

Decomposition:

$$D^{\alpha}_{*0} T(t) = -\lambda T(t),$$

solution: $T(t) = E_{\alpha,1}(-\lambda t^{\alpha})$

$$L(X)(x) = \lambda X(x), \qquad X(x) = 0 \text{ for } x \in \partial G.$$

classical eigenvalue problem for elliptic operator L

Construction of the Solution

Consequences:

- eigenvalue problem (L + BC) is positive definite and self-adjoint
- eigenvalue problem has countably many eigenvalues λ_j, $j \in \mathbb{N}$, all of which are in $(0, \infty)$ and have finite multiplicity (WLOG $0 < \lambda_1 \leq \lambda_2 \leq \lambda_3 \leq \ldots$)
- denote the eigenfunction corresponding to λ_j by X_j
- any function of the form $u_j(x,t) = c_j E_{\alpha,1}(-\lambda_j t^\alpha) X_j(x)$ satisfies the PDE and the boundary condition

Theorem

If ∂G is smooth then the function

$$u(x,t) = \sum_{j=1}^{\infty} (u_0, X_j) E_{\alpha,1}(-\lambda_j t^\alpha) X_j(x)$$

is a formal solution to the fractional initial-boundary value problem. Under suitable assumptions, it is even an actual solution.

Comparison to Classical Case

assumption: compatibility of IC & BC; smoothness of given data

Classical parabolic IBVP ($\alpha = 1$):

infinitely differentiable w.r.t. t on $[0, T]$

$$u(x,t) = \sum_{j=1}^{\infty} (u_0, X_j) \exp(-\lambda_j t) X_j(x)$$

exponential decay as $t \to \infty$

Fractional parabolic IBVP ($0 < \alpha < 1$):

infinitely differentiable w.r.t. t on $(0, T]$; not differentiable at 0

$$u(x,t) = \sum_{j=1}^{\infty} (u_0, X_j) E_{\alpha,1}(-\lambda_j t^{\alpha}) X_j(x)$$

algebraic decay $\sim t^{-\alpha}$ as $t \to \infty$

- Behaviour with respect to x (smoothness etc.): same in both cases
- Behaviour with respect to t: remember $\lambda_j > 0$ for all j

References

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Thank you for your attention!

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