Stochastic Models for Fractional Subdiffusion with Reactions and Forcing

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Rudyard Kipling (1885)

*Four out from crow-clump: three left; nine out; two right; three back; two left; fourteen out; two left; seven out; one left; nine back; two right; six back; four right; seven back.*
1. RANDOM WALKS - DIFFUSION
2. ANOMALOUS DIFFUSION
3. CONTINUOUS TIME RANDOM WALKS
4. SUBDIFFUSION WITH REACTIONS AND FORCING
5. GENERALIZED MASTER EQUATION DERIVATION
6. FUTURE DIRECTIONS
Uhlenbeck and Ornstein (Phys. Rev., 1930)

In the theory of Brownian motion the first concern has always been the calculation of the mean square displacement of the particle, because this could immediately be observed.

\[ \langle \Delta X^2(t) \rangle = \langle (X(t) - \langle X(t) \rangle)^2 \rangle \sim t \]
First Steps

Bachelier (*PhD, Théorie de la Speculation*, 1900) first consideration of a stochastic process in continuous time

\[ \int_0^\infty x p(x, t) \, dx = k \sqrt{t} \]

Pearson (*Nature*, 1905): \( n \) steps, 2-dim off-lattice, probability to be between \( r \) and \( r + dr \) from starting point

Rayleigh (*Nature*, 1905):

\[ P = \frac{2}{n} e^{-\frac{r^2}{n}} r \, dr \]

\[ \langle r^2 \rangle = n \]


\[ \frac{\partial f}{\partial t} = D \frac{\partial^2 f}{\partial x^2}, \quad \langle x^2(t) \rangle = 2Dt, \quad D = \left( \frac{RT}{6N \pi a \eta} \right) = \left( \frac{k_B T}{\gamma} \right) \]

Langevin (*Comptes Rendues Acad. Sci.*, 1908)

..a demonstration that is infinitely more simple ..

\[ m \frac{d^2 x}{dt^2} = F(t) - \gamma \frac{dx}{dt} \]

\[ \langle F(t) \rangle = 0, \langle F(0)F(t) \rangle = D \delta(t), \langle x(t)F(t) \rangle = 0, \quad \langle x^2 \rangle \sim 2Dt, \quad D = \frac{k_B T}{\gamma} \]
Diffusion with Reactions and Forcing

Diffusion with Reactions

Fisher (\textit{Ann. Eug.}, 1937); Kolmogorov et al (\textit{Moscow Math. Bull.}, 1937)

\[
\frac{\partial n}{\partial t} = D \frac{\partial^2 n}{\partial x^2} + \lambda n(1 - n), \quad \frac{\partial n}{\partial t} = D \frac{\partial^2 n}{\partial x^2} + f(n(x, t))
\]

Diffusion with Forcing

Fokker (\textit{Ann. Phys.}, (1914), Planck (1917), Kolmogorov (1931)

\[
\frac{\partial \rho}{\partial t} = \frac{\partial^2}{\partial x^2} (D(x, t)\rho(x, t)) - \frac{\partial}{\partial x} (b(x, t)\rho(x, t))
\]

Smoluchowski (\textit{Ann. Phys.},1915)

\[
\frac{\partial \rho}{\partial t} = D \frac{\partial^2 \rho}{\partial x^2} - \frac{\partial}{\partial x} (F(x, t)\rho(x, t)), \quad F(x, t) = -\frac{\partial V(x, t)}{\partial x}
\]

Ito stochastic equation \(dX_t = \mu(X_t, t) \, dt + \sigma \, dW_t\)
Klafter (Physics World, 2005)

*the clear picture that has emerged over the last few decades is that although these phenomena are called anomalous, they are abundant in everyday life: anomalous is normal!*

\[
\langle \Delta X^2(t) \rangle = \langle (X(t) - \langle X(t) \rangle)^2 \rangle \sim t
\]
### Anomalous Diffusion

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Subdiffusion


molecules in spiny nerve cells – Santamaria et al *Neuron* 2006

telomeres in mammalian cells – Bronstein et al *Phys Rev Letts* (2009)


lipid molecules in lipid bilayers – Akimoto et al *Phys Rev Letts* (2011)


potassium channels in the brain – Weigel et al *PNAS* (2011)
Subdiffusion in Nerve Cells

Spiny dendrites, Computational Neurobiology and Imaging Centre, Mount Sinai School of Medicine, New York

Scaled Brownian Motion Diffusion Equation


- Time dependent diffusion coefficient $D(t) = \alpha t^{\alpha - 1} D_0$, $0 < \alpha < 1$

$$\frac{\partial \rho}{\partial t} = \alpha t^{\alpha - 1} D_0 \frac{\partial^2 \rho}{\partial x^2}$$

- Non-Markovian probability density function

$$\rho(x, t) = \frac{1}{\sqrt{4\pi D_0 t^\alpha}} \exp \left( -\frac{x^2}{4D_0 t^\alpha} \right)$$

  Rescaled Gaussian

- Anomalous subdiffusion

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} x^2 \rho(x, t) \, dx = 2D_0 t^\alpha = 2D_0 t^{2H}$$

  $H$ Hurst exponent

- Note $D(t) = 0D_t^{1-\alpha} (\Gamma(\alpha + 1)D_0)$

$$0D_t^{1-\alpha} y(t) = \frac{d}{dt} 0I_t^{\alpha} y(t)$$
Dissipative memory kernel

\[ m \frac{dv}{dt} = F(t) - m \int_0^t \gamma(t - t') v(t') \, dt' \]

\( \langle F(t) \rangle = 0 \quad \langle F(0)F(t) \rangle = D_\alpha t^{-\alpha} \) coloured noise

Equilibrium fluctuation-dissipation theorem

\( \langle F(t)F(0) \rangle = mk_B T \gamma(t) \quad \Rightarrow \quad \gamma(t) = \frac{D_\alpha}{mk_B T} t^{-\alpha} \)

\( \Rightarrow m \frac{dv}{dt} = F(t) - \frac{D_\alpha}{k_B T} 0D_t^{\alpha-1} v(t) \quad 0 < \alpha < 1 \)

The probability density function for trajectories satisfies the fractional Brownian motion diffusion equation.
Rescaled Gaussian

\[ \rho(x, t) = \frac{1}{\sqrt{4\pi D_0 t^\alpha}} \exp \left( -\frac{x^2}{4D_0 t^\alpha} \right) \]

Non-Markovian

\[ P(T > t + s | T > s) > P(T > t) \]

Ergodic

\[ \langle x^2(t) \rangle_E = \langle x^2(t) \rangle_T = 2D_0 t^\alpha \]

Ensemble Average

\[ \langle x^2(t) \rangle_E = \langle (x(t) - x(0))^2 \rangle \]

Moving Time Average

\[ \langle x^2(t) \rangle_T = \frac{1}{T-t} \int_0^{T-t} (x(t + t') - x(t'))^2 \, dt' \]
Banjo Patterson (The Bulletin, 1892)

*It was the man from Ironbark who struck the Sydney town, he wandered over street and park, he wandered up and down. He loitered here, he loitered there, till he was like to drop, until at last in sheer despair, he sought a barbers shop.*
Continuous Time Random Walks – CTRWs

**Standard Random Walk**

The step length is a fixed distance \( \Delta x \)

Steps occur at discrete times separated by a fixed time interval \( \Delta t \)

**Continuous Time Random Walk**

Montroll & Weiss, 1965; Scher & Lax, 1973

The step length is selected at random from a step length probability density \( \lambda(x) \)

Steps occur after a waiting time selected at random from a waiting time probability density \( \psi(t) \)
Standard Diffusion or Fractional Subdiffusion


Assume $\lambda(x) = \lambda(-x)$ with finite variance $\sigma^2 = \int x^2 \lambda(x) \, dx$
Gaussian $\lambda(x) = \frac{1}{\sqrt{2\pi}\sigma^2} \exp\left(-\frac{x^2}{2\sigma^2}\right)$ or n.n. $\lambda(x) = \delta(x \pm \Delta x)$.

- Markovian exponential waiting time density
  \[ \psi(t) = \frac{1}{\tau} \exp\left(-\frac{t}{\tau}\right) \]

  \[ \frac{\partial \rho}{\partial t} = D \frac{\partial^2 \rho}{\partial x^2}, \quad D = \frac{\sigma^2}{2\tau} \]

- Non Markovian power law tail waiting time density
  Pareto $\psi(t) \sim \frac{\alpha \tau^\alpha}{t^{1+\alpha}} \quad t \in [\tau, \infty], \quad 0 < \alpha < 1$
  Mittag-Leffler $\psi(t) = -\frac{d}{dt} E_\alpha\left(-\frac{t^\alpha}{\tau^\alpha}\right) \quad E_\alpha(z) = \sum_{n=0}^{\infty} \frac{z^n}{\Gamma(\alpha n+1)}$
  Scalas, Gorenflo, Mainardi (2004)

  \[ \frac{\partial \rho}{\partial t} = 0D_{t}^{1-\alpha} D_\alpha \frac{\partial^2 \rho}{\partial x^2}, \quad D_\alpha = \frac{\sigma^2}{2\tau^\alpha \Gamma(1-\alpha)} \quad 0 < \alpha < 1 \]
Subordinated probability density function
\( G(x, t) \) – Green’s solution time fractional subdiffusion
\( G^*(x, t) \) – Green’s solution standard diffusion

\[
G(x, t) = \int_0^\infty G^*(x, \tau) T(\tau, t) \, d\tau
\]

\( \mathcal{L}(T(\tau, t)) = \hat{T}(\tau, u) = u^{\alpha-1} e^{-\tau u^\alpha} \) \( t \) – physical time, \( \tau \) – operational time

scales as number of steps

Subordinated stochastic process

\[
X(t) = Y(S_t) \quad dY(\tau) = (2D_\alpha)^{\frac{1}{2}} dB(\tau)
\]

\( S_t \) inverse-time \( \alpha \)-stable subordinator \( S_t = \inf\{\tau : U(\tau) > t\} \)
random time the process \( U(\tau) \) exceeds \( t \)
\( U(\tau) \) \( \alpha \)-strictly increasing \( \alpha \)-stable Levy process with p.d.f. \( g(t, \tau) \)

\[
\mathcal{L}[g(t, \tau)] = e^{-\tau u^\alpha} \quad g(t, \tau) = \frac{1}{\tau^{1/\alpha}} g\left( \frac{t}{\tau^{1/\alpha}} \right) \]
self-similar
Non-Gaussian

Non-Markovian

\[ P(T > t + s | T > s) > P(T > t) \]

Non-Ergodic

\[ \langle x^2(t) \rangle_E \neq \langle x^2(t) \rangle_T \]

Subdiffusive

\[ \langle x^2(t) \rangle = \frac{2D_\alpha}{\Gamma(1 + \alpha)} t^\alpha \]
Subdiffusion and Reaction Terms are not Simply Additive

Linear reaction kinetics

\[ \frac{dn}{dt} = -kn \quad \Rightarrow \quad n(x, t) = n(x, 0)e^{-\int_0^t k \, dt'} \]

Straightforward generalization A.

\[ \frac{\partial n}{\partial t} = D_{\alpha} \frac{\partial^{1-\alpha}}{\partial t^{1-\alpha}} \left( \frac{\partial^2 n}{\partial x^2} \right) - kn \]


\[ n(x, t) = \frac{1}{\sqrt{4\pi D_{\alpha} t^\alpha}} \sum_{j=0}^{\infty} \frac{(-kt)^j}{j!} H_{1,2}^{2,0} \left[ \frac{x^2}{4D_{\alpha} t^\alpha} \right] (1 - \frac{\alpha}{2} + j, \alpha) \bigg|_{(0, 1)} \bigg( \frac{1}{2} + j, 1 \bigg) \]

The solution is not strictly positive for all \( x \) and \( t \).
Subdiffusion and Reaction Terms are not Subordinated

\[
\frac{dn}{dt} = -kn \quad \Rightarrow \quad n(x, t) = n(x, 0) e^{-\int_0^t k \, dt'}
\]

Straightforward generalization B.

\[
\frac{\partial n}{\partial t} = \frac{\partial^{1-\alpha}}{\partial t^{1-\alpha}} \left( D_\gamma \frac{\partial^2 n}{\partial x^2} - kn \right)
\]

This models the case when a fixed fraction of walkers is removed at the start of each waiting time (Henry, Langlands, Wearne, *Phys. Rev. E*, 2006)

\[
n(x, t) = (1 - k) \Phi(t) n(x, 0) + \sum_{x'} \int_0^t n(x', t')(1 - k) \psi(t - t') \lambda(x - x') \, dt'
\]
Subdiffusion and Reaction Terms are Entwined

\[ \frac{dn}{dt} = -kn \quad \Rightarrow \quad n(x, t) = n(x, 0)e^{-\int_0^t k dt'} \]


\[ n(x, t) = e^{-kt}\Phi(t)n(x, 0) + \sum_{x'} \int_0^t n(x', t')e^{-k(t-t')}\psi(t-t')\lambda(x-x')dt' \]

\[ \frac{\partial n}{\partial t} = D_\gamma e^{-kt} \frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}} \left( e^{kt} \frac{\partial^2 n}{\partial x^2} \right) - kn \]


\[ \frac{\partial n}{\partial t} = \int_0^t K(t-t')e^{-k(t-t')}\frac{\partial^2 n}{\partial x^2} dt' - kn \]
Subdiffusion and Nonlinear Reactions


Nonlinear reaction kinetics

\[
\frac{dn}{dt} = r(n)n \quad \Rightarrow \quad n(x, t) = n(x, 0)e^{\int_0^t r(n(x, t')) dt'}
\]

Master equation

\[
\frac{\partial n}{\partial t} = \int_0^t K(t - t') \left( \int_{-\infty}^{+\infty} n(x', t')e^{\int_{t'}^t r(n(x', t'')) dt''} \lambda(x - x') \, dx' \right) \, dt' + r(n)n, \quad K(t) = \mathcal{L}^{-1} \left[ \frac{\mathcal{L} \left[ \psi(t) \right]}{\mathcal{L} \left[ \Phi(t) \right]} \right]
\]


\[
\frac{\partial n}{\partial t} = \phi(x, t) K_0 D_t^{1-\gamma} \frac{\partial^2}{\partial x^2} \left( \frac{n}{\phi(x, t)} \right) + \frac{1}{\phi(x, t)} \frac{d\phi}{dt} n
\]

\[
\phi(x, t) = \exp \int_{t'}^t r(n(x, t'')) dt''
\]
Subdiffusion and External Forces run on Different Clocks


\[ \frac{\partial \rho(x, t)}{\partial t} = 0D_t^{1-\alpha} \left[ \kappa_\alpha \frac{\partial^2}{\partial x^2} - \frac{1}{\eta_\alpha} \frac{\partial}{\partial x} F(x) \right] \rho(x, t) \]


\[ X(t) = Y(S_t) \quad dY(\tau) = \frac{1}{\eta} F(Y(\tau)) \, d\tau + (2\kappa)^{\frac{1}{2}} dB(\tau) \]

Simply time-subordinated to the solution of the standard Fokker-Planck equation.


\[ \frac{\partial \rho(x, t)}{\partial t} = \left[ \kappa_\alpha \frac{\partial^2}{\partial x^2} - \frac{1}{\eta_\alpha} F(t) \frac{\partial}{\partial x} \right] 0D_t^{1-\alpha} \rho(x, t) \]


\[ X(t) = Y(S_t) \quad dY(\tau) = \frac{1}{\eta} F(U(\tau)) \, d\tau + (2\kappa)^{\frac{1}{2}} dB(\tau) \]

Not simply time-subordinated to the solution of the standard Fokker-Planck equation.
Space and Time Dependent Forcing

Weron, Magdziarz, Weron, (Phys. Rev. Letts, 2008)

\[ X(t) = Y(S_t) \begin{pmatrix} dY(\tau) \\ dZ(\tau) \end{pmatrix} = \begin{pmatrix} F(Y(\tau), Z(\tau)) \\ 0 \end{pmatrix} d\tau + \begin{pmatrix} (2\kappa)^{\frac{1}{2}} dB(\tau) \\ dU(\tau) \end{pmatrix} \]

\[ S_t = \inf\{\tau : U(\tau) > t\} \]


\[ \frac{\partial \rho(x, t)}{\partial t} = \left[ \kappa_\alpha \frac{\partial^2}{\partial x^2} - \frac{1}{\eta_\alpha} \frac{\partial}{\partial x} F(x, t) \right] 0D_t^{1-\alpha} \rho(x, t) \]

\[ \kappa_\alpha = A_\alpha \frac{\Delta x^2}{2^{2\alpha}} \quad \eta_\alpha = (2\beta \kappa_\alpha)^{-1} \]
Reactions: Birth and Death Processes

\[ \omega(x, t)\delta t + o(\delta t) \] probability of a particle dying in \((t, t + \delta t)\)

\[ \eta(x, t)\delta t + o(\delta t) \] probability of a particle being created in \((t, t + \delta t)\)

\[ \theta(x, t, s) = e^{-\int_s^t \omega(x, t')dt'} \] probability of particle surviving to time \(t\)

\[ \theta(x, t, s) = \theta(x, t', s)\theta(x, t, t') \] useful identity

Example

\[ A + B \rightleftharpoons_{k_1}^{k_{-1}} A + 2B, \quad B \rightarrow_{k_2}^{} C \]

\[ \frac{dc_B}{dt} = k_1c_Ac_B - k_2c_B - k_{-1}c_Ac_B^2 \]

\[ \omega_B(x, t)\delta t = (k_2 + k_{-1}c_Ac_B)\delta t \]

\[ \eta_B(x, t)\delta t = k_1c_Ac_B\delta t \]
Forcing: Biased Jumps

\[ \Psi(x, x', t, t') = \lambda(x, x', t) \psi(x', t - t') \]

transition probability for a particle at \( x' \) at time \( t' \) to jump to \( x \) at time \( t \)

\[ \lambda(x, x', t) \] jump density allowing for space and time dependent forcing

\[ \sum_x \lambda(x, x', t) = 1 \quad \text{for fixed } x' \text{ and } t \]

\[ \psi(x', t - t') \] waiting time density allowing for spatially dependent trapping

\[ \int_{t'}^{\infty} \psi(x', t - t') \, dt = 1 \quad \text{for fixed } x' \text{ and } t'. \]
Single Particle Master Equation

Probability per unit time for a walker **to arrive** at point \( x \) at time \( t \) given that it was at point \( x_0 \) at time 0

\[
q(x, t|x_0, 0) = \delta_{x,x_0} \delta(t - 0^+) + \sum_{x'} \int_0^t \psi(x, x', t, t') \theta(x', t', t) q(x', t'|x_0, 0) dt'
\]

Probability per unit time for a walker **to leave** point \( x \) at time \( t \) given that it was at point \( x_0 \) at time 0

\[
i(x, t|x_0, 0) = \int_0^t \psi(x, t - t') \theta(x', t', t) q(x', t'|x_0, 0) dt'
\]

Probability of a particle **to be** at point \( x \) at time \( t \)

\[
\rho(x, t|x_0, 0) = \int_0^t \Phi(x, t - t') \theta(x, t, t') q(x, t'|x_0, 0) dt'
\]

Jump survival probability

\[
\Phi(x, t - t') = 1 - \int_0^{t-t'} \psi(x, t'') dt''
\]
Single Particle Master Equation

Useful separation

\[ q(x, t|x_0, 0) = \delta_{x,x_0} \delta(t - 0^+) + q^+(x, t|x_0, 0) \]

Differentiation of \( \rho(x, t) \)

\[
\frac{\partial \rho(x, t|x_0, 0)}{\partial t} = q^+(x, t|x_0, 0) - \delta_{x,x_0} \theta(x, t, 0) \psi(x, t) \\
- \int_0^t q^+(x, t'|x_0, 0) \theta(x, t, t') \psi(x, t - t') dt' \\
- \omega(x, t) \rho(x, t|x_0, 0)
\]

Formally equivalent to a flux balance

\[
\frac{\partial \rho(x, t|x_0, 0)}{\partial t} = q^+(x, t|x_0, 0) - i(x, t|x_0, 0) - \omega(x, t) \rho(x, t|x_0, 0)
\]
Single Particle Master Equation

Useful identity

$$\frac{\rho(x, t|x_0, 0)}{\theta(x, t, 0)} = \int_0^t \frac{q(x, t'|x_0, 0)}{\theta(x, t', 0)} \Phi(x, t-t') dt'$$

Simplification

$$\frac{\partial \rho(x, t|, x_0, 0)}{\partial t} = \sum_{x'} \lambda(x, x', t) \int_0^t K(x', t-t') \rho(x', t'|x_0, 0) \theta(x', t, t') dt'$$
$$- \int_0^t K(x, t-t') \rho(x, t'|x_0, 0) \theta(x, t, t') dt'$$
$$- \omega(x, t) \rho(x, t|x_0, 0)$$

Kernel

$$\hat{K}(x, s) = \frac{\hat{\psi}(x, s)}{\hat{\Phi}(x, s)}$$
Ensemble Master Equation

Ensemble of particles, created and destroyed by reactions, subject to an external force field, newly created particles draw a new waiting time

Density of particles at $x$ at time $t$

$$u(x, t) = \sum_{x_0} \int_0^t \rho(x, t|x_0, t_0)\eta(x_0, t_0)dt_0$$

Differentiation, using the single particle master equation,

$$\frac{\partial u(x, t)}{\partial t} = \sum_{x'} \lambda(x, x', t) \int_0^t K(x', t - t')\theta(x', t, t')u(x', t')dt'$$

$$- \int_0^t K(x, t - t')\theta(x, t, t')u(x, t')dt' - \omega(x, t)u(x, t) + \eta(x, t)$$

Angstmann, Donnelly, Henry *Mathematical Modelling of Natural Phenomenon* (2013)
Special Cases

I) Reduction to Checkin, Gorenflo, Sokolov (2005)
\[ \psi(x, t - t') \] spatially inhomogeneous
\[ \lambda(x, x', t) = \frac{1}{2}(\delta(x, x - \Delta x) + \delta(x, x + \Delta x)) \] no forcing
\[ \theta(x, t, t') = 0, \omega(x, t) = 0, \eta(x, t) = 0 \] no reactions

\[ \int_0^t K(x, t - t') \rho(x, t') dt' = \frac{d}{dt} \int_0^t M(x, t - t') \rho(x, t') dt', \quad \hat{M}(x, s) = \frac{\hat{\psi}(x, s)}{s \Phi(x, s)} \]

\[ \psi(x, t - t') = \psi(t - t') \] spatially homogeneous
\[ \lambda(x, x', t) = \frac{1}{2}(\delta(x, x - \Delta x) + \delta(x, x + \Delta x)) \] no forcing
\[ \theta(x, t, t') = e^{-k(t-t')}, \omega(x, t) = k, \eta(x, t) = 0 \] no births

III) Reduction to Fedotov (2010)
\[ \psi(x', t - t') = \psi(t - t') \] spatially homogeneous
\[ \lambda(x, x', t) = \frac{1}{2}(\delta(x, x - \Delta x) + \delta(x, x + \Delta x)) \] no forcing
\[ \theta(x, t, t') = e^{-\int_t^{t'} r^+(u(x, t'')) dt''}, \omega(x, t) = r^-(u(x, t)), \eta(x, t) = r^+(u(x, t)) u(x, t) \]
One dimensional lattice, biased nearest neighbour jumps

\[ \lambda(x_i, x_{i-1}, t) = p_r(x_{i-1}, t) \] probability to jump to the right from \( x_{i-1} \)

\[ \lambda(x_i, x_{i+1}, t) = p_\ell(x_{i+1}, t) \] probability to jump to the left from \( x_{i+1} \)

\[
\frac{\partial u(x_i, t)}{\partial t} = \int_0^t K(x_{i-1}, t - t') p_r(x_{i-1}, t) \theta(x_{i-1}, t, t') u(x_{i-1}, t') dt' + \int_0^t K(x_{i+1}, t - t') p_\ell(x_{i+1}, t) \theta(x_{i+1}, t, t') u(x_{i+1}, t') dt' - \int_0^t K(x_i, t - t') \theta(x_i, t, t') u(x_i, t') dt' - \omega(x_i, t) u(x_i, t) + \eta(x_i, t)
\]
Biased Jumps

\[ F(x, t) = -\frac{\partial V(x, t)}{\partial x} \]

near thermodynamic equilibrium, Boltzmann weights

\[ p_r(x_i, t) = \frac{e^{-\beta V(x_{i+1}, t)}}{e^{-\beta V(x_{i+1}, t)} + e^{-\beta V(x_{i-1}, t)}}, \]
\[ p_\ell(x_i, t) = \frac{e^{-\beta V(x_{i-1}, t)}}{e^{-\beta V(x_{i+1}, t)} + e^{-\beta V(x_{i-1}, t)}} \]

Continuum limit, \( x_i = x, \ x_{i\pm 1} = x \pm \Delta x \), Taylor series expansions in \( x \), retaining leading order terms in \( \Delta x \)

\[
\frac{\partial u(x, t)}{\partial t} = \frac{\Delta x^2}{2} \frac{\partial^2}{\partial x^2} \int_0^t \theta(x, t, t') u(x, t') K(x, t - t') \, dt' \\
- \beta \Delta x^2 \frac{\partial}{\partial x} \left( F(x, t) \int_0^t \theta(x, t, t') u(x, t') K(x, t - t') \, dt' \right) \\
- \omega(x, t) u(x, t) + \eta(x, t)
\]
Special Case - Fractional Dispersion

Reduction to Sokolov, Klafter (2006)

*Field-Induced Dispersion in Subdiffusion*

\[ \psi(x, t - t') = \psi(t - t') \] spatially homogeneous

\[ F(x, t) = F(t) \] time dependent forcing

\[ \theta(x, t, t') = 0, \omega(x, t) = 0, \eta(x, t) = 0 \] no reactions

\[ \int_0^t K(x, t - t') \rho(x, t') \, dt' = \frac{d}{dt} \int_0^t M(x, t - t') \rho(x, t') \, dt', \quad \hat{M}(x, s) = \frac{\hat{\psi}(x, s)}{s \hat{\phi}(x, s)} \]
\( \psi(x, t) = \gamma(x)e^{-\gamma(x)t} \) exponential waiting time density \( K(x, t) = \gamma(x)\delta(t) \)

\[
\frac{\partial u(x, t)}{\partial t} = \frac{\partial^2}{\partial x^2} (D(x)u(x, t)) - \frac{\partial}{\partial x} \left( \frac{1}{\zeta(x)} F(x, t)u(x, t) \right) - \omega(x, t)u(x, t) + \eta(x, t)
\]

\[
D(x) = \lim_{\Delta x, \langle \tau(x) \rangle \to 0} \frac{\Delta x^2}{2\langle \tau(x) \rangle}, \quad \zeta(x) = \lim_{\Delta x, \langle \tau(x) \rangle \to 0} \frac{2\langle \tau(x) \rangle}{\beta \Delta x^2}
\]

\( D(x) \) and \( \zeta(x) \) finite and differentiable w.r.t. \( x \)
Fractional Fokker-Planck Equation with Reactions

Angstmann, Donnelly, Henry *Mathematical Modelling of Natural Phenomenon* (2013)

Spatially dependent Pareto waiting time density

\[
\psi(x, t) = \begin{cases} 
\frac{\alpha(x) t^\alpha(x)}{t^{1+\alpha(x)}} & t \in [\tau, \infty), \\
0 & t \in [0, \tau)
\end{cases}
\text{ for } 0 < \alpha(x) < 1
\]

\[
\int_0^t K(x, t - t') y(x, t') \, dt' \approx \frac{1}{\tau^{\alpha(x)} \Gamma(1 - \alpha(x))} D_t^{1-\alpha(x)} y(x, t), \quad \theta(x, t, t') = \frac{\theta(x, t, 0)}{\theta(x, t', 0)}
\]

\[
\frac{\partial u(x, t)}{\partial t} = \frac{\partial^2}{\partial x^2} \left( D_{\alpha(x)} \theta(x, t, 0) D_t^{1-\alpha(x)} \left[ \frac{u(x, t)}{\theta(x, t, 0)} \right] \right) \\
- \frac{\partial}{\partial x} \left( \frac{1}{\zeta_{\alpha(x)}} F(x, t) \theta(x, t, 0) D_t^{1-\alpha(x)} \left[ \frac{u(x, t)}{\theta(x, t, 0)} \right] \right) - \omega(x, t) u(x, t) + \eta(x, t)
\]

\[
D_{\alpha(x)} = \lim_{\Delta x^2, \tau \to 0} \frac{\Delta x^2}{2 \tau^{\alpha(x)} \Gamma(1 - \alpha(x))}, \quad \zeta_{\alpha(x)} = \lim_{\Delta x^2, \tau \to 0} \frac{\tau^{\alpha(x)} \Gamma(1 - \alpha(x))}{\beta \Delta x^2}
\]
No reactions $\theta(x, t, t') = 0, \omega(x, t) = 0, \eta(x, t) = 0$


*From continuous time random walks to the fractional Fokker-Planck equation*

$$F(x, t) = F(x), \quad \alpha(x) = \alpha$$

II) Reduction to Sokolov, Klafter (2006)

*Field-Induced Dispersion in Subdiffusion*

$$F(x, t) = F(t), \quad \alpha(x) = \alpha$$


*Fractional Fokker-Planck Equations for Subdiffusion with Space- and Time-Dependent Forces*

$$F(x, t) = F(x, t), \quad \alpha(x) = \alpha$$


\[
\frac{\partial n}{\partial t} = e^{kt} D_t^{1-\alpha} \left( e^{-kt} \kappa_\alpha \frac{\partial^2 n}{\partial x^2} \right) - \chi_\alpha \frac{\partial}{\partial x} \left( \frac{\partial c}{\partial x} e^{kt} D_t^{1-\alpha} (e^{-kt} n) \right) + kn
\]

In progress, nonlinear reaction diffusion equations with chemotaxis and anomalous diffusion
Fractional electro-diffusion

Collaboration – CNIC Mount Sinai School of Medicine New York


- Fractional cable equation

\[
\frac{\partial V}{\partial T} = 0D_{T}^{1-\gamma} \frac{\partial^2 V}{\partial X^2} - \mu^2 0D_{T}^{1-\kappa}(V - i_e r_m)
\]

- In progress, fractional compartmental models for whole neurons
\[ \frac{du(w_j, t)}{dt} = \int_0^t \left[ \sum_{i=1}^J K(w_i, t - t') \lambda(w_i, w_j) \theta(w_i, t, t') u(w_i, t') - K(w_j, t - t') \theta(w_j, t, t') u(w_j, t') \right] dt' \]

\[-\beta(w_j, t) u(w_j, t) + \eta(w_j, t).\]

Reaction survival function
\[ \theta(w_i, t, t') = e^{-\int_{t'}^t \beta(w_i, t'') dt''} \]

Standard diffusion
\[ \psi(w_j, t) = \alpha(w_j) e^{-\alpha(w_j) t} \]
\[ \Rightarrow K(w_j, t) = \alpha(w_j) \delta(t) \]
\[ \lambda(w_i, w_j) = \frac{A_{ij}}{k_i} \]
CTRW with Forcing on Networks

\[
\frac{du(v_i, t)}{dt} = \sum_{j=1}^{J} \lambda(v_i|t, v_j) \int_{t_0}^{t} K(t - t'|v_j)u(v_j, t') \, dt' - \int_{t_0}^{t} K(t - t'|v_i)u(v_i, t') \, dt'
\]

Self-chemotactic like forcing

Bias in the jump density dependent on the concentration of particles on neighbouring vertices

\[
\lambda(v_i|t, v_j) = \frac{A_{j,i}e^{\beta u(v_i,t)}}{\sum_{k=1}^{J} A_{j,k}e^{\beta u(v_k,t)}}
\]

Steady state pairing patterns, concentration localized in distinct pairs of adjacent vertices
Thank You
Appendix: Stochastic Subdiffusion Process


\[ X(t) = Y(S_t) \left( \begin{array}{c} dY(\tau) \\ dZ(\tau) \end{array} \right) = \left( \begin{array}{c} F(Y(\tau), Z(\tau)) \\ 0 \end{array} \right) d\tau + \left( \begin{array}{c} (2\kappa)^{\frac{1}{2}} dB(\tau) \\ dU(\tau) \end{array} \right) \]

\[ S_t = \inf\{\tau : U(\tau) > t\} \]

\[ q_t(y, z) \text{ p.d.f. of } (Y_t, Z_t) \text{ – generalized stochastic process, Levy noise} \]

\[ \frac{\partial}{\partial t} q_t(y, z) = \kappa \frac{\partial^2}{\partial y^2} q_t(y, z) - \frac{\partial}{\partial y} \left( \frac{F(y, z)}{\eta} q_t(y, z) \right) - D_z^\alpha q_t(y, z) \]

\[ \rho_t \text{ p.d.f. of } X(t) \text{ – compensation formula} \]

\[ \int_{I} p_t(x) \, dx = \int_{0}^{\infty} \, dt' \int_{I} \, dy \int_{0}^{t} \, dz \, q_{t'}(y, z) \frac{(t-z)^{-\alpha}}{\Gamma(1-\alpha)} \]

\[ p_t(x) = \int_{0}^{\infty} \, dt' \, 0_{t'^{1-\alpha}} q_{t'}(x, t) \]

\[ \frac{\partial}{\partial t} p_t(x) = \kappa \frac{\partial^2}{\partial x^2} 0D_t^{1-\alpha} p_t(x) - \frac{\partial}{\partial x} \left( \frac{F(x, t)}{\eta} 0D_t^{1-\alpha} p_t(x) \right) \]