From discrete time random walks to numerical methods for fractional order differential equations

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Never Stand Still

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Collaborators

Everything

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Fractional Fokker-Planck equation and reaction sub-diffusion

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Fractional SIR models

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References

C. N. Angstmann et al. A discrete time random walk model for anomalous diffusion, *J. Comput. Phys.* (2015), doi:10.1016/j.jcp.2014.08.003

C. N. Angstmann et al. From stochastic processes to numerical methods: A new scheme for solving reaction subdiffusion fractional partial differential equations *J. Comput. Phys.* (2016) doi:10.1016/j.jcp.2015.11.053

C. N. Angstmann et al. A fractional order recovery SIR model from a stochastic process. *Bulletin of Mathematical Biology*, (2016)
doi:10.1007/s11538-016-0151-7

The Idea

Consider a particle that is undergoing a random walk.

At every point in time we have a probability distribution for the location of the particle.

This probability distribution evolves in time according to a governing equation.

The Idea

For a discrete time system the governing equation is a difference equation.

For a continuous time system the governing equation is a differential equation.

If we construct a sequence of discrete time random walks that tend towards a continuous time random walk, then we will also have a sequence of difference equations that tend to the differential equation.

Advantages

As the approximation is always a governing equation for the random walk then we have some guarantees about its behavior.

- In the absence of reactions we know that the particle is not created nor destroyed, so the scheme must conserve mass.
- The approximation is always a finite distance from the solution of the differential equation.

We can use the tools of stochastic processes on the numerical method.

Example: A Biased Random Walk

The governing equation for finding the particle undergoing a biased random walk at position *x*, at time *t* is:

$$X(x,t) = p_r(x-\Delta x, t-\Delta t)X(x-\Delta x, t-\Delta t) + p_l(x+\Delta x, t-\Delta t)X(x+\Delta x, t-\Delta t)$$

Taking the "diffusion" limit of this process gives a Fokker-Planck equation as the governing equation:

$$\frac{\partial X(x,t)}{\partial t} = D\frac{\partial^2 X(x,t)}{\partial x^2} - 2D\beta\frac{\partial}{\partial x}\left(f(x,t)X(x,t)\right)$$

Where

$$D = \lim_{\Delta x, \Delta t \to 0} \frac{\Delta x^2}{2\Delta t} \qquad f(x,t) = \lim_{\Delta x \to 0} \frac{p_r(x,t) - p_l(x,t)}{\beta \Delta x}$$

Boltzmann weights

Boltzmann weights are taken for the jump probabilities.

$$p_r(x,t) = \frac{\exp(-\beta V(x+\Delta x, t))}{\exp(-\beta V(x+\Delta x, t)) + \exp(-\beta V(x-\Delta x, t))} \qquad f(x,t) = -\frac{\partial V(x,t)}{\partial x}$$

This guarantees that $0 < p_r(x,t) < 1$ for all Δx.

Example: Burgers Equation

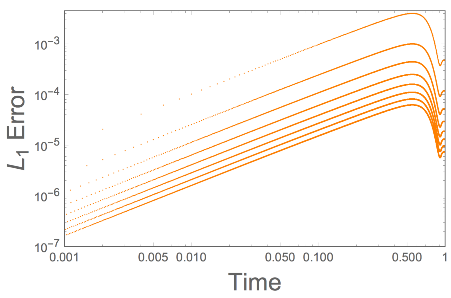
Burgers equation,

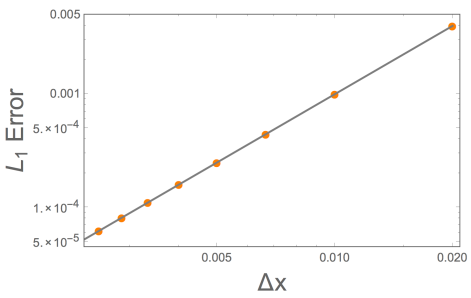
$$\frac{\partial u(x,t)}{\partial t} = \nu \frac{\partial^2 u(x,t)}{\partial x^2} - u(x,t)\frac{\partial u(x,t)}{\partial x}$$

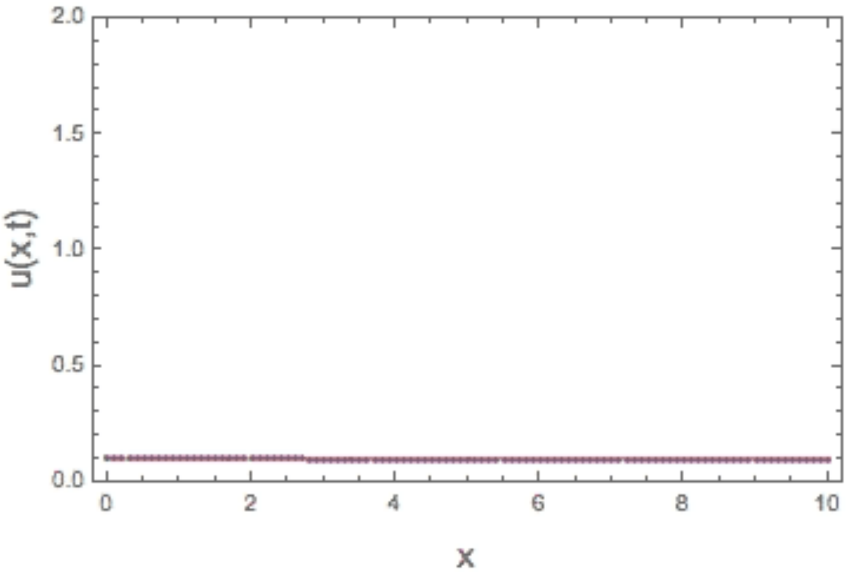
can be approximated by

$$u(x,t) = \frac{u(x-\Delta x, t-\Delta t)}{1+\exp(\frac{\Delta x}{8\nu}(u(x-2\Delta x, t-\Delta t) + 2u(x-\Delta x, t-\Delta t) + u(x, t-\Delta t)))}$$
$$+ \frac{u(x-\Delta x, t-\Delta t)}{1+\exp(\frac{\Delta x}{8\nu}(u(x-2\Delta x, t-\Delta t) + 2u(x-\Delta x, t-\Delta t) + u(x, t-\Delta t)))}$$

Example: Burgers Equation







Fractional Fokker-Planck Equation

The fractional Fokker-Planck equation is

$$\frac{\partial u(x,t)}{\partial t} = D\frac{\partial^2}{\partial x^2}\left({}_0\mathcal{D}_t^{1-\alpha}\left(u(x,t)\right)\right) - 2D\beta\frac{\partial}{\partial x}\left(f(x,t)\ {}_0\mathcal{D}_t^{1-\alpha}\left(u(x,t)\right)\right)$$

Where ${}_0\mathcal{D}_t^{1-\alpha}\left(u(x,t)\right)$ is the Riemann-Liouville fractional derivative defined by

$${}_0\mathcal{D}_t^{1-\alpha}\left(u(x,t)\right) = \frac{1}{\Gamma(\alpha)}\frac{\partial}{\partial t}\int_0^t (t-v)^{\alpha-1}u(x,v)\,dv \qquad 0<\alpha<1$$

This equation is typically derived from the limit of a Continuous Time Random Walk.

Fractional Fokker-Planck Equation

To find approximations for a fractional Fokker-Planck equation we need to use a different discrete time random walk.

We modify the random walk by letting the particle wait for a random number of time steps before jumping.

This introduces a waiting time probability distribution, $\psi(n)$.

By choosing an appropriate heavy tailed distribution the governing equations will limit to the fractional Fokker-Planck equation.

Discrete Time Random Walk

For such a random walk the governing equation is, in general,

$$u(x,n\Delta t) = u(x,(n-1)\Delta t) + p_r(x-\Delta x,(n-1)\Delta t)\sum_{m=0}^{n-1} K(n-m)u(x-\Delta x,m\Delta t)$$
$$+ p_l(x+\Delta x,(n-1)\Delta t)\sum_{m=0}^{n-1} K(n-m)u(x+\Delta x,m\Delta t) - \sum_{m=0}^{n-1} K(n-m)u(x,m\Delta t)$$

Where *K(n)* is the memory kernel associated with the waiting time probability distribution. It is defined through it's Z transform with

$$\mathcal{Z}\{K(n)\} = \frac{\mathcal{Z}\{\psi(n)\}}{\mathcal{Z}\{\phi(n)\}}$$

Where $\phi(n)$ is the probability that the particle has not jumped by the n time step since arriving at the site.

Sibuya Distribution

To limit to the fractional Fokker-Planck equation we take the Sibuya waiting time distribution,

$$\psi(n) = (-1)^{n+1} \frac{\Gamma(\alpha+1)}{\Gamma(n+1)\Gamma(\alpha-n+1)} \qquad \phi(n) = \prod_{m=1}^{n} \left(1 - \frac{\alpha}{m}\right)$$

for $0 < \alpha < 1$ and $n > 0$. This gives a tractable memory kernel

$$K(n) = \delta_{n,1} + \frac{\Gamma(n-1+\alpha)}{\Gamma(\alpha-1)\Gamma(n+1)}$$

Example: Fractional Diffusion Equation

The simplest fractional example is the fractional diffusion equation, which just *f*(*x*,*t*)=0. Taking $\alpha = \frac{4}{5}$, and $D = 1$.

$$\frac{\partial \rho(x,t)}{\partial t} = \mathcal{D}_t^{1-\frac{4}{5}} \frac{\partial^2 \rho(x,t)}{\partial x^2}$$

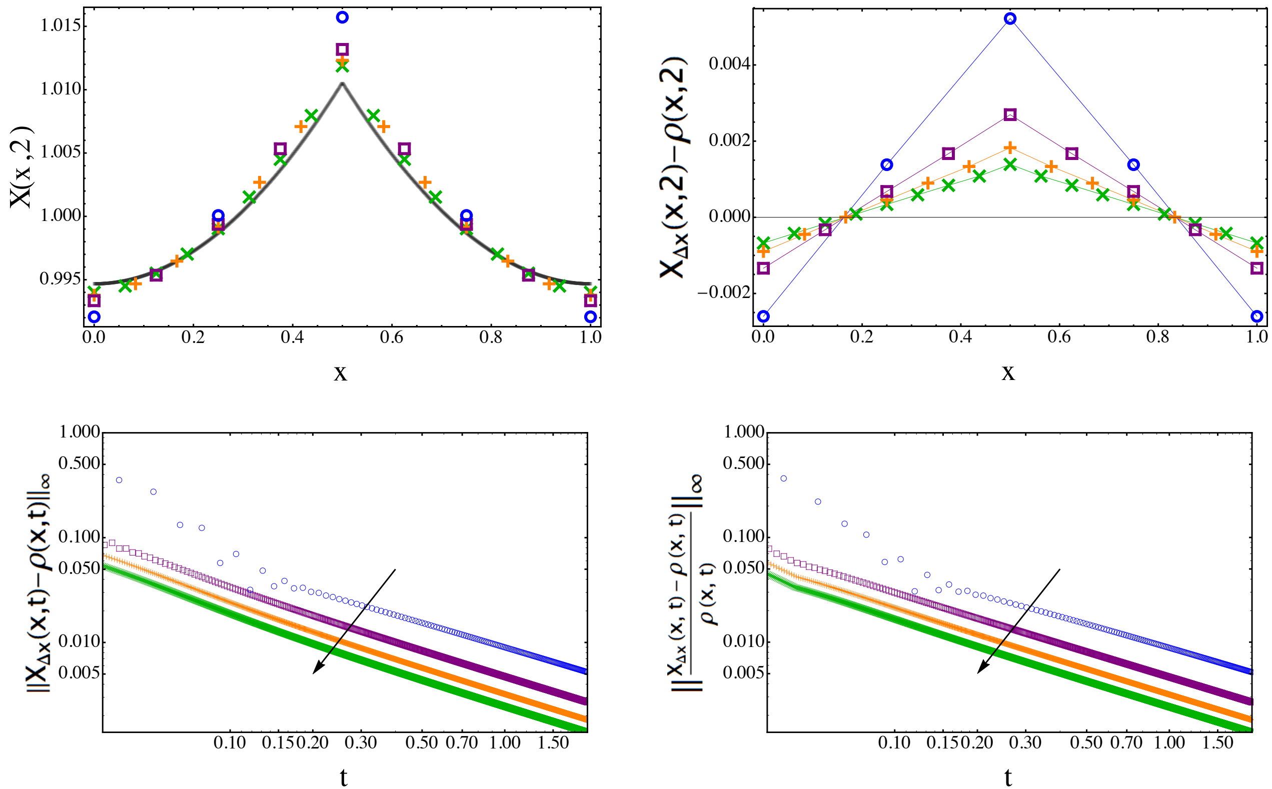
With zero flux boundaries

$$\left.\frac{\partial \rho(x,t)}{\partial x}\right|_{x=0} = 0 \qquad \left.\frac{\partial \rho(x,t)}{\partial x}\right|_{x=1} = 0$$

and the initial condition

$$\rho(x,0) = \delta(x - \tfrac{1}{2})$$

Example: Fractional Diffusion Equation



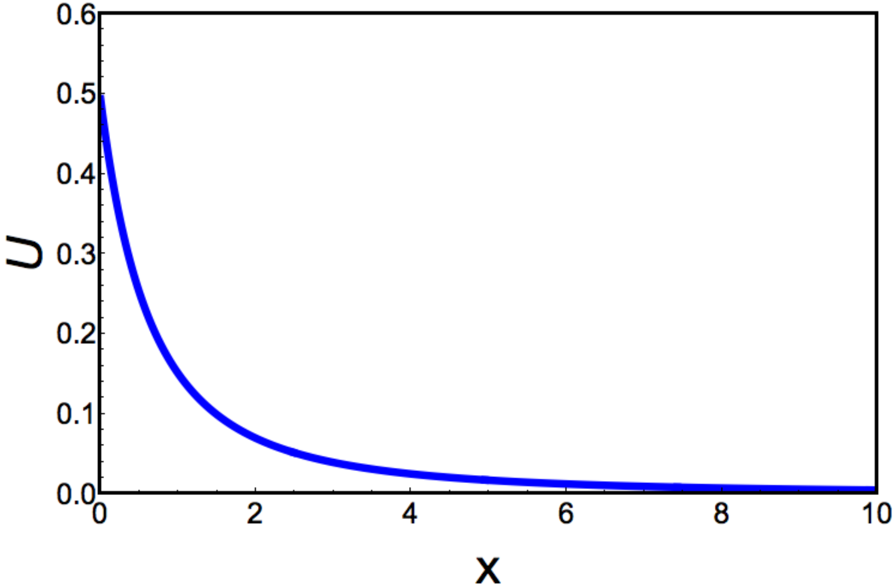
Reaction sub-diffusion equations

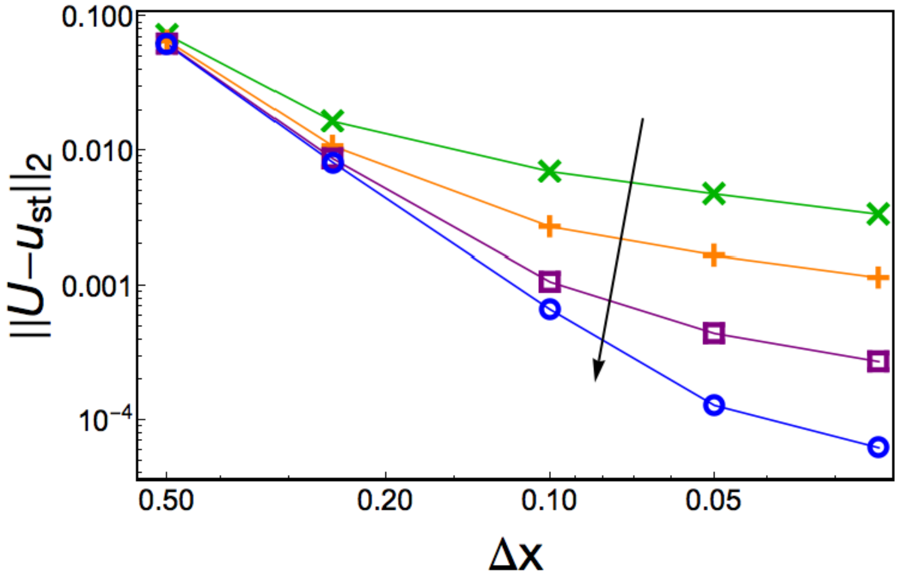
Schemes for more complicated equations can also be found with this approach. For example the reaction sub-diffusion equation.

$$\frac{\partial u(x,t)}{\partial t} = D\frac{\partial^2}{\partial x^2}\left[\exp\left(-\int_0^t d(x,t')dt'\right)\mathcal{D}_t^{1-\alpha}\left[\exp\left(\int_0^t d(x,t')dt'\right)u(x,t)\right]\right] - d(x,t)u(x,t) + b(x,t)$$

The stochastic process used is slightly different in this case. We take an ensemble of randomly walking and reacting particles.

Non-linear morphogen death rates on semi-infinite domain





$$\frac{\partial u(x,t)}{\partial t} = \frac{\partial^2}{\partial x^2}\left[D e_0^{-\int_0^t ku(x,s)ds} \mathcal{D}_t^{1-\alpha}\left(e^{\int_0^t ku(x,s)ds} u(x,t)\right)\right] - ku(x,t)^2$$

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