Fractional Dynamics for Quantum Random Walks

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Outline

1. An Introduction to Fractional Calculus
2. Background on QRWs and Our Fractional Model
3. A Numerical Method to Solve the Fractional QRW Problem
4. An Optimization Algorithm to Determine the Fractional Order in Time

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Fractional Calculus: Fourier Approach

Fractional derivatives typically appear in the form of the fractional Laplacian $(-\Delta)^s$ or the fractional time derivative ∂_t^α.

- The Fractional Laplacian $(-\Delta)^s$ of order $0 < s < 1$ is defined as:

$$(-\Delta)^s u = \mathcal{F}^{-1}(|\xi|^{2s}\mathcal{F}(u))$$

  for u defined on $\mathbb{R}^n$.

- While the fractional time derivative can be defined as

$$\partial_t^\alpha u = \mathcal{F}^{-1}((i\omega)^\alpha \mathcal{F}(u))$$

From Fourier to Pointwise Definition of Caputo Derivative

Starting from

$$\partial_t^\alpha u = \mathcal{F}^{-1}((i\omega)^\alpha \mathcal{F}(u)),$$

we get

$$\partial_t^\alpha u = \mathcal{F}^{-1}\left(\frac{\Gamma(1-\alpha)}{\Gamma(1-\alpha)}(i\omega)^{\alpha-1}(i\omega)\mathcal{F}(u)\right)$$

$$= \mathcal{F}^{-1}\left(\mathcal{F}\left(\frac{1}{\Gamma(1-\alpha)t^\alpha}\right)\mathcal{F}(\partial_t u)\right) = \mathcal{F}^{-1}\left(\mathcal{F}\left(\frac{1}{\Gamma(1-\alpha)t^\alpha} * \partial_t u(t)\right)\right)$$

where $*$ denotes convolution. We arrive at

$$\partial_t^\alpha u = \frac{1}{\Gamma(1-\alpha)}\int_{-\infty}^{t} \frac{\partial_t u(y)}{(t-y)^\alpha}\, dy$$

which is the Marchaud fractional derivative. Setting u to be constant on $(-\infty, 0)$ recovers the Caputo fractional derivative of order $0 < \alpha < 1$

$$\partial_t^\alpha u(t) = \frac{1}{\Gamma(1-\alpha)}\int_{0}^{t} \frac{\partial_t u(y)}{(t-y)^\alpha}\, dy$$

Random Walk View of Fractional Derivatives

Fractional Laplacian:

- $(-\Delta)^s$ comes from a **long jump** random walk
- Intuitively, this means that the fractional Laplacian is nonlocal in space, i.e. is able to look farther around itself

Fractional Time Derivative:

- ∂_t^α with order $0 < \alpha < 1$ comes from a random walk with **time delays**
- Time delays, τ, behave like $\frac{\alpha A_\alpha}{\Gamma(1-\alpha)\tau^{(1+\alpha)}}$, where A_α is a constant depending on α
- The fractional time derivative is then nonlocal in time. The derivative has memory effects.

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Our Application Area: Quantum Random Walks (QRW)

Motivation:

- QRWs are essential tools for quantum computing
- Have applications in algorithm design and can be a universal model of computation (Venegas-Andraca 2012)

QRWs:

- A quantum walk is described by a tensor product of two vectors $\psi_c \otimes \psi_p = \sum_{i=-N}^{N} (a_i w_0 + b_i w_1) \otimes v_i$
- The basis vectors v_i correspond to positions along a line
- The probability of being at position i is $P(i) = |a_i|^2 + |b_i|^2$
- Coin and shift operators evolve the state
- We are specifically studying a **Hadamard walk**, whose coin operator is the matrix $C = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$

Quantum Walk vs Classical Walk

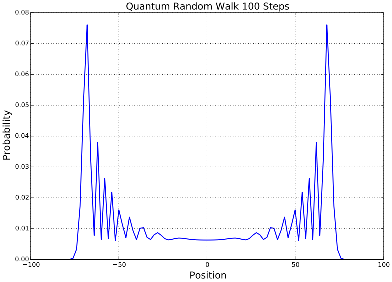


Figure: Quantum Random Walk

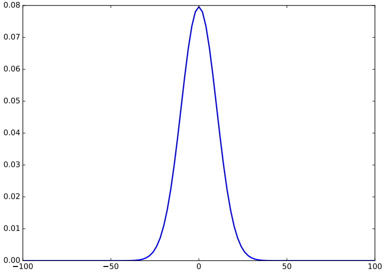
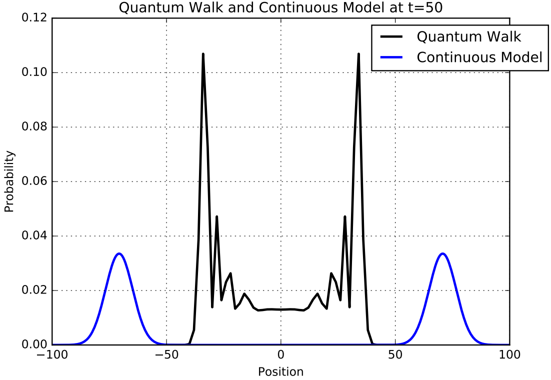


Figure: Classical Random Walk

From Blanchard and Hongler (2004)

As $t \to \infty$, the following PDE describes the probability density, u

$$\frac{\partial}{\partial t} u(t,x) = \frac{1}{2}\frac{\partial^2}{\partial x^2} u(t,x) - \frac{\partial}{\partial x}[\tanh(x) u(t,x)]$$
$$u(0,x) = \delta(x), \lim_{x \to \pm\infty} u(t,x) = 0$$



- The peaks of the continuous model move too quickly relative to the QRW
- A fractional model could slow these peaks down and provide a better fit for the QRW

Our Fractional Model

Why the Fractional Derivative Makes Sense:

- Comes from the random walk view of fractional derivatives
- Fractional derivative means time delays in the walk

Our Model

$$\partial_t^\alpha u(t,x) = \frac{1}{2}\frac{\partial^2}{\partial x^2}u(t,x) - \frac{\partial}{\partial x}[\tanh(x)u(t,x)]$$
$$u(0,x) = \delta(x), \lim_{x\to\pm\infty} u(t,x) = 0$$

∂_t^α is the Caputo fractional derivative of order $0 < \alpha \leq 1$.

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Numerical Method

Our numerical method does the following:

- Solves the fractional PDE on the domain $(0, T) \times \Omega$ with $\Omega = (-\frac{L}{2}, \frac{L}{2})$ and homogenous Dirichlet boundary conditions with L sufficiently large
- spectral method in space
- L^1 finite difference scheme in time

By taking the sine transform, we get the PDE in the frequency domain

$$\partial_t^\alpha \mathcal{F}_s\{u\} = -\frac{\pi^2\omega^2}{2L^2}\mathcal{F}_s\{u\} + \frac{\pi\omega}{L}\mathcal{F}_c\{\tanh(x)u\}$$

where

- $\mathcal{F}_s$ denotes a sine transform
- $\mathcal{F}_c$ denotes a cosine transform
- ω is the frequency variable

L^1-scheme for time discretization (Lin and Xu 2007)

We use the definition of the Caputo Fractional derivative

$$\partial_t^\alpha u(t,x) = \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{u_t(y,x)}{(t-y)^\alpha} dy$$

By using a backwards difference approximation for $u_t(y,x)$, the discretization of $\partial_t^\alpha u(x,t)$ at time $t_k = k\tau$ with time step τ is

$$\begin{aligned}
\partial_t^\alpha u(x, t_{k+1}) &\approx \frac{1}{\Gamma(1-\alpha)} \sum_{\ell=0}^{k} \int_{t_\ell}^{t_{\ell+1}} \frac{u_{\ell+1} - u_\ell}{\tau(t_{k+1} - y)^\alpha}\, dy \\
&\approx \frac{1}{\Gamma(1-\alpha)} \sum_{\ell=0}^{k} \frac{u_{\ell+1} - u_\ell}{\tau} \int_{t_\ell}^{t_{\ell+1}} \frac{1}{(t_{k+1} - y)^\alpha}\, dy \\
&\approx \frac{1}{\Gamma(2-\alpha)} \sum_{\ell=0}^{k} \frac{u_{\ell+1} - u_\ell}{\tau^\alpha} a_{k-\ell}
\end{aligned}$$

Recall the PDE in the frequency domain:

$$\partial_t^\alpha \hat{u}_{k+1} = -\frac{\pi^2\omega^2}{2L^2}\hat{u}_{k+1} + \frac{\pi\omega}{L}\mathcal{F}_c\{\tanh(x)u\}$$

where $\hat{u}_{k+1}$ denotes $\mathcal{F}_s\{u\}$ at $t = (k+1)\tau$. If we apply the L^1 scheme to the LHS we get a forward time marching scheme

$$\hat{u}_{k+1} = C_2\left[\frac{\pi\omega}{L}\mathcal{F}_c\{\tanh(x)u_{k+1}\} + C_1\left(\hat{u}_k - \sum_{\ell=0}^{k-1}(\hat{u}_{\ell+1} - \hat{u}_\ell)a_{k-\ell}\right)\right]$$

$C_1 = (\Gamma(2-\alpha)\tau^\alpha)^{-1}$ and $C_2 = \left(C_1 + \frac{\pi^2\omega^2}{2L^2}\right)^{-1}$,

- We cannot calculate $\mathcal{F}_c\{\tanh(x)u\}$ directly
- A nested fixed point iteration (FPI) can bypass this issue

Our Approximation Converges with Time and Space Refinements

We have an analytical solution when $\alpha = 1$, below are L_2 errors of our method on the domain $(0, 10) \times (-200, 200)$.

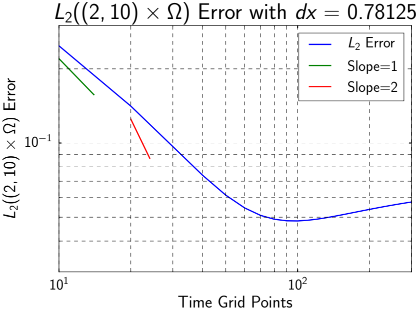
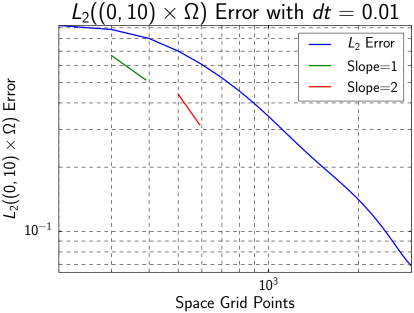


Figure: The convergence rate with respect to space refinements is between 1 and 2



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Optimization

The functional we are minimizing is

$$E[\alpha] = \frac{1}{2} \int_0^T \int_\Omega (u_\alpha - q)^2 + \gamma \frac{1}{(1-\alpha)\alpha}$$

- u_α is the cumulative probability distribution of the solution to our PDE model with the derivative order α
- q is the linear interpolant of the quantum random walk cumulative probability distribution
- The far right term will prevent the optimization process from going outside the interval $(0, 1)$, with $\gamma \leq 1$

Optimization Method

Using a right hand rule Riemann sum approximation of the integral, we approximate the gradient of our functional.

$$E'[\alpha] \approx h\tau \sum_i \sum_j \left[(u_\alpha(t_i, x_j) - q(t_i, x_j)) \frac{d}{d\alpha} u_\alpha(t_i, x_j) \right] + \gamma \frac{2\alpha - 1}{(1-\alpha)^2 \alpha^2}$$

- h is the spatial step size
- τ is the time step size
- $\frac{d}{d\alpha} u_\alpha(t_i, x_j)$ will be a backward difference approximation

Using this approximation for the gradient, we'll use a gradient descent method to find optimal α

Optimization Numerical Results

T	10	20	30	40	50	60	70
Optimal α	0.645	0.701	0.724	0.742	0.754	0.763	0.771

Table: Optimal α values at differing T values

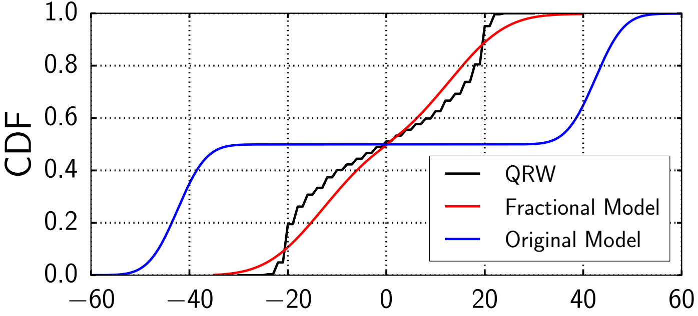

Figure: Comparison of CDFs from the QRW and the fractional model with the optimal α value from when $T = 30$

Conclusion

We have done the following

- Enriched Blanchard and Hongler's (2004) model by introducing a fractional derivative in time
- Provided a numerical scheme to solve the fractional model and provided a method to find optimal α

Future Work:

- Analysis of our numerical scheme for our problem (error estimates and stability)
- Analysis of the optimization problem to determine the fractional time order α

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