Balancing the Nodes: Solving the Fractional Diffusion Equation with Contour Integration

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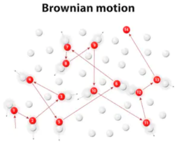
Introduction

Motivation

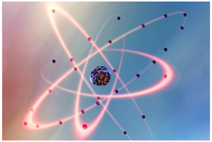
Probability: Continuous-time random walk [1]

$$(\partial_t)^\beta P(x,t) = D_{\alpha,\beta}(\partial_x)^\alpha P(x,t).$$



Quantum Mechanics: Fractional Schrödinger equation [2]

$$i\hbar\partial_t\psi(\mathbf{r},t) = D_\alpha(-\hbar\Delta)^\alpha\psi(\mathbf{r},t) + V(\mathbf{r},t)\psi(\mathbf{r},t).$$



Fractional Diffusion Equation

The key to solving the two equations above is accurately solving the fractional diffusion equation:

$$\begin{cases} \partial_t u + (-\partial_x^2)^\alpha u = 0 & \text{in } \mathbb{R} \times [0, \infty), \\ u = f & \text{on } \mathbb{R} \times \{t = 0\}, \end{cases}$$

where $\alpha \in (0, 1]$.

Rewriting Solution Using Spectral Measure

The solution to the fractional diffusion equation is described through an operator exponential

$$u(x,t) = e^{-(-\partial_x^2)^\alpha t} f(x),$$

which can be written in terms of an integral over a spectral measure:

$$\exp(-(-\partial_x^2)^\alpha t) f = \left[\int_0^\infty e^{-\lambda^\alpha t} d\mathcal{P}_{\mathcal{L}}(\lambda)\right] f.$$

Approximating the Spectral Measure

To evaluate this spectral measure, we use Stone's formula:

$$\lim_{\epsilon\to 0}\int_0^\infty \frac{1}{\pi}\mathrm{Im}(\mathcal{R}_{\mathcal{L}}(\lambda+i\epsilon)f)e^{-\lambda^\alpha t}d\lambda = \left[\int_0^\infty e^{-\lambda^\alpha t}d\mathcal{P}_{\mathcal{L}}(\lambda)\right]f.$$

After fixing some small ϵ, the integral on the left-hand side can be evaluated using a quadrature rule.

Problems with this method

$$\lim_{\epsilon \to 0} \int_0^\infty \frac{1}{\pi} \mathrm{Im}(\mathcal{R}_{\mathcal{L}}(\lambda + i\epsilon) f) e^{-\lambda^\alpha t} d\lambda = \left[\int_0^\infty e^{-\lambda^\alpha t} d\mathcal{P}_{\mathcal{L}}(\lambda) \right] f.$$

There is a delicate balance to set the parameter ϵ :

- On one hand, we want ϵ to be small to ensure that the limit is close enough to the spectral integral.
- On the other hand, we can not pick ϵ to be too small, in which case the originally smooth integrand becomes less regular.

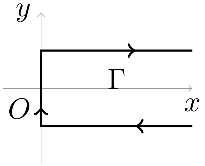
Question: Can we develop a method that does not involve choosing such an ϵ?

Creating the Contour

Hankel Contour

- Consider a different version of Stone's formula

$$\lim_{\epsilon \to 0} \frac{1}{2\pi i}(\mathcal{R}_{\mathcal{L}}(x+i\epsilon) - \mathcal{R}_{\mathcal{L}}(x-i\epsilon))f = \mathcal{P}_{\mathcal{L}}f.$$



  - Integrating both sides gives

$$\exp\left(-(-\partial_x^2)^{\alpha}t\right)f = \frac{1}{2\pi i}\int_{\Gamma} e^{-z^{\alpha}t}\mathcal{R}_{\mathcal{L}}(z)f\,dz$$

where Γ is a Hankel contour that winds from $+\infty - 0i$ in the lower half-plane, around 0, and back to $+\infty + 0i$.

Three Concrete Contours

In practice, we consider three concrete examples of contours: [4]

- **Parabola**: $z(\theta) = a + b\theta^2 + ic\theta \ (a \leq 0,\ c > 0)$
- **Hyperbola**: $z(\theta) = a\sin(b + ci\theta) - a\sin(b)$
- **Cotangent**: $z(\theta) = a + b(\theta\cot(c\theta) + di\theta)$

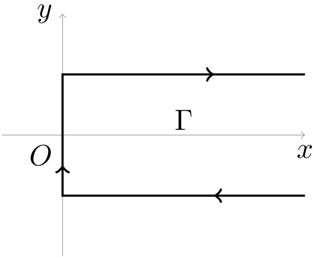


Figure: Hankel Contour

$\Longrightarrow$

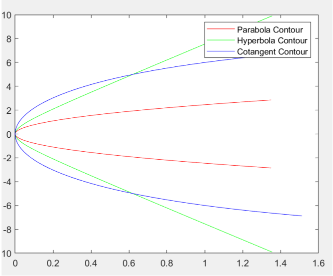


Figure: Concrete Contours

Summary of Contour Design

- **Error estimate**: With suitable choice of parameters, these three contours have an exponential decay of error [4]:
  - Parabola $O(2.85^{-N})$; Hyperbola $O(3.20^{-N})$; Cotangent $O(3.89^{-N})$
- **Problem**: The above bounds do not hold for our equation, which has a branch point at 0.
- **Next Step**: Find the optimal choice of quadrature rule that gives best approximation while minimizing the effect of branch point.

Quadrature Rule and Discretization Size

Quadrature Rule for the New Contours

If we have a quadrature rule with nodes $\{\theta_1, \ldots, \theta_n\}$ and weights $\{w_1, \ldots, w_n\}$, we have the approximation

$$\exp\left(-(-\partial_x^2)^\alpha t\right) f \approx \sum_{l=1}^{n} w_l e^{-z(\theta_l)^\alpha t} \cdot [\mathcal{R}_{\mathcal{L}}(z(\theta_l))f] \cdot z'(\theta_l)$$

Thus, we would like to approximate the following:

- The exponential $e^{-z(\theta_l)^\alpha t}$.
- The resolvent $\mathcal{R}_{\mathcal{L}}(z(\theta_l))f = (\mathcal{L} - z(\theta_l))^{-1} f$.

Balancing Distance to Origin

- **Exponential**: Let $\alpha = \frac{1}{2}$, $k = 0$ and $t = 1$. In this case, we want to approximate $e^{-z(\theta_l)^{\frac{1}{2}}} = e^{-\sqrt{z(\theta_l)}}$.
- **Problem**: The derivative of the above expression

$$\frac{d}{d\theta_l}(e^{-\sqrt{z(\theta_l)}}) = \frac{1}{2\sqrt{z(\theta_l)}} e^{-\sqrt{z(\theta_l)}} z'(\theta_l)$$

  blows up when $z(\theta_l) \approx 0$.
- **Clustering Near Origin**: Since the above function varies faster around $z(\theta_l)$, we need more quadrature nodes clustered around the origin.

Balancing Distance to Origin, Continued

- **Resolvent**: $\mathcal{R}_{\mathcal{L}}(z(\theta_l)) = (\mathcal{L} - z(\theta_l))^{-1}$.
- **Problem**: As $z(\theta_l)$ gets closer to 0, the resolvent will have larger condition number, and this may result in inaccurate approximations.
- **Solution**:
  - We pick an even number of quadrature nodes symmetric across the real axis, to avoid the singularity at $z(\theta_l) = 0$.
  - We impose a fixed threshold $\epsilon' > 0$ such that all quadrature nodes satisfy $|z(\theta_l)| > \epsilon'$.

Balancing the Discretization Size

There is also a balance involved in determining the number of Fourier modes (or discretization size):

- We need **sufficiently large** number of Fourier modes to accurately approximate the differential operator.
- We **can not have too many** Fourier modes, as the discretization of the resolvent $\mathcal{R}_{\mathcal{L}}(z) = (\mathcal{L} - z)^{-1}$ will have a large determinant when we have larger discretization size.

Summary of our Expectations for the Quadrature Rule

- **Position**: We pick an even number of nodes symmetric to the real axis, with a threshold bounding it away from 0.
- **Clustering**: The quadrature nodes are more clustered in regions closer to the origin.
- **Discretization**: We choose the best discretization size that balances approximation power and complexity of finding the resolvent.

Doubly Exponential Quadrature

- To cluster nodes more rapidly at the origin, we try a new quadrature rule called "doubly exponential quadrature" [3].
- **Idea**: Take lots of quadrature points near 0!
- **Reparametrization Map**: Define $f : [0, \infty) \to [0, 1]$ by

$$f(s) = 1 - \tanh\left(\frac{\pi}{2}\sinh(s)\right)$$

with $f(0) = 1$, and $f(\infty) = 0$.

Re-Parametrization

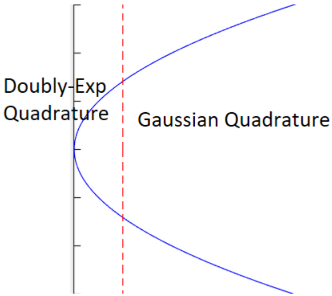


Figure: After re-parametrization

Re-parametrization

- We first define a general quadrature rule on θ, and pick the index k such that Re $\theta_k \leq 1$ and Re $\theta_{k+1} > 1$.
- Integration on interval $[1, \infty)$ follows the original quadrature rule.
- Integration on interval $[0, 1]$ is done using doubly exponential quadrature rule, where we reparametrize by

$$\theta(s) = \theta_k \left(1 - \tanh(\frac{\pi}{2} \sinh(s))\right),$$

which changes that part of integral to

$$\int_0^\infty \frac{1}{\pi} \text{Im } (e^{\sqrt{z(\theta(s))}t}(\mathcal{L} - z(\theta(s)))^{-1} f(x)) z'(\theta(s)) \theta'(s) ds.$$

Experiments

Experiment Setting

In the experiments below, we will solve the fractional diffusion equation

$$\begin{cases} \partial_t u + (-\partial_x^2)^{\frac{1}{2}} u = 0 & \text{in } \mathbb{R} \times [0, \infty), \\ u = \frac{1}{1+x^2} & \text{on } \mathbb{R} \times \{t = 0\}, \end{cases}$$

Using Fourier transforms, we can obtain its analytical solution

$$u(x,t) = \sqrt{\frac{\pi}{2}} \int_{\mathbb{R}} e^{-|y| + 2\pi i x y - (4\pi^2 y^2 + k^2)^{\frac{1}{2}} t} dy,$$

which we compare our method to after numerical integration of the above integral for $t = 1$.

Experiment 1: Contour Comparison

We first run experiments to verify the performance of our method on the three contours (parabola, hyperbola, and the cotangent curve). The contours have the following parameters:

- **Parabola**: $z(\theta) = 1 + 0.15\theta^2 + 0.95i\theta$
- **Hyperbola**: $z(\theta) = \sin(0.15 + 0.95i\theta) - \sin(0.15)$
- **Cotangent**: $z(\theta) = 0.75 - 1.5(\theta\cot(2\theta) + 1.25i\theta)$

We evaluate the parabola and the hyperbola contours on $\theta \in [0, 30]$ and the cotangent contour on $\theta \in [0, \pi]$.

Experiment 1: Contour Comparison

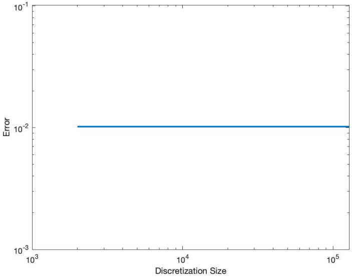
All experiments in this section are run with 1500 Fourier modes and 900 quadrature nodes.

Type of Contour	Maximum Error
Parabola Contour	0.008
Hyperbola Contour	0.0079
Cotangent Contour	0.0012

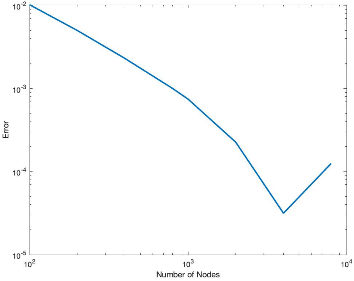
Table: Comparing different contours under the given parameters

The cotangent contour gives the best approximation.

Experiment 2: Gaussian Quadrature



Nodes set at 100



Discretization size set at 1500

Experiment 3: Doubly-Exponential Quadrature

We truncate the number of quadrature nodes so that they are at least 2×10^{-8} away from origin (note that we say "first ___" to indicate how many nodes are actually used).

Discretization Size	Number of Nodes	Maximum Error
10^3	500, first 350	$1.76 * 10^{-4}$
10^4	500, first 350	$5.29 * 10^{-5}$
800	40000, first 28000	$1.20 * 10^{-5}$
600	40000, first 28000	$6.98 * 10^{-6}$
600	50000, first 35000	$6.51 * 10^{-6}$

Table: Tests across the cotangent contour showing increase in accuracy with greater number of nodes and smaller discretization size

Future Work

Motivation, Revisited

Probability: Continuous-time random walk [1]

$$(\partial_t)^\beta P(x,t) = D_{\alpha,\beta}(\partial_x)^\alpha P(x,t).$$

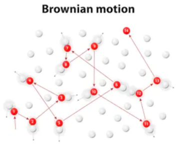


Figure: Caption

Quantum Mechanics: Fractional Schrödinger equation [2]

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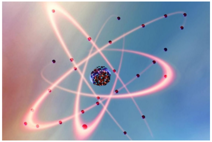

Figure: Caption

Next Steps: Fractional Time Equations

- Motivated by continuous-time random walks, consider the model problem:

$$\begin{cases} (\partial_t)^\beta u + (-\partial_x^2)^\alpha u = 0 & \text{in } \mathbb{R} \times [0, \infty), \\ u = f & \text{on } \mathbb{R} \times \{t = 0\}, \end{cases}$$

- The solution is given by

$$u(x,t) = \left[\int_0^\infty E_\beta \left(-\lambda^\alpha t^\beta \right) d\mathcal{P}_{\mathcal{L}}(\lambda) \right] f,$$

where our previous exponential $e^{-z^\alpha t}$ is replaced by the Mittag-Leffler function E_β:

$$E_\beta \left(-z^\alpha t^\beta \right) = \sum_{l=0}^{\infty} \frac{\left(-z^\alpha t^\beta \right)^l}{\Gamma(\beta l + 1)}.$$

Next Steps: Anomalous Reaction-Diffusion Equation

- Motivated by Schrödinger equations, we consider the model problem:

$$\begin{cases} \partial_t u + (-\partial_x^2)^\alpha u = V(x)u & \text{in } \mathbb{R} \times [0, \infty), \\ u = f & \text{on } \mathbb{R} \times \{t = 0\}, \end{cases}$$

- We rewrite equation in the form

$$\partial_t u = V(x)u - (-\partial_x^2)^\alpha u = (A + R)u = Fu$$

  where $Au = V(x)u$ is a simple operator, and $Ru = -(-\partial_x^2)^\alpha u$ is a complicated operator.
- Then we can apply an operator splitting scheme to this problem.

References

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[3] M. Mori and M. Sugihara. The double-exponential transformation in numerical analysis. *Journal of Computational and Applied Mathematics*, 127(1-2):287–296, 2001.

[4] L. N. Trefethen, J. A. C. Weideman, and T. Schmelzer. Talbot quadratures and rational approximations. *BIT Numerical Mathematics*, 46(3):653–670, 2006.