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Analysis of Tempered Fractional Operators

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Abstract: Tempered fractional operators are useful in models for subsurface transport and diffusion due to their ability to capture anomalous diffusion: a behavior which the classical partial differential equation models cannot describe. We analyze tempered fractional operators within the nonlocal vector calculus framework in order to assimilate them to the rigorous mathematical structure developed for nonlocal models. First, we show they are special instances of generalized nonlocal operators in correspondence of a proper choice of nonlocal kernels [D'Elia, Gulian, Olson, & Karniadakis, 2020]. Then, we work towards showing tempered fractional operators are equivalent to truncated fractional operators. These truncated operators are useful because they are less computationally intensive than the tempered operators.

Figure 1. Sketching out some ideas for proofs. Photo credit: Hayley Olson.

Analysis of Tempered Fractional Operators

Introduction

This research project focuses on some aspects of the nonlocal vector calculus, firstly introduced in [4] and further developed in [3]. In particular, we use the nonlocal calculus framework to analyze tempered fractional operators [8] and include them in the rigorous mathematical background we developed. My interest in this project stems from the research I am working on in my graduate program. I currently study nonlocal operators and was intrigued by the opportunity to apply that background to a new problem.

Description of Research Project

The purpose of this research project is to include tempered fractional models in the unified nonlocal calculus framework that we developed in [3]. A unified calculus that includes fractional models as special cases will impact both the nonlocal and fractional communities, who will be able to benefit from each other's results. Also, a unified framework will facilitate the process of learning a mathematical model for an intrinsically nonlocal phenomenon. An important feature of fractional models is their ability to capture anomalous diffusion (i.e. the mean square displacement in a diffusion process is proportional to time to a fractional power, instead of being linear with respect to time). While these operators have been used for decades in subsurface diffusion and transport [2, 5, 6, 9, 10], they have recently found application in turbulence [7]. However, their improved predictive capability comes at the price of incredibly high computational cost – this in particular motivates us to find an equivalent alternative through the nonlocal calculus framework that is computationally cheaper.

This project has a double sided objective. First, we show that the tempered fractional models are a special instance of generalized nonlocal operators for a proper choice of the *equivalence nonlocal kernel* observed in [3]. Second, we propose an operator that acts equivalently to tempered fractional operators, but can be computed at a cheaper cost. Our conjecture is that fractional truncated operators (fractional operators whose kernels have support over a finite region, as opposed to tempered operators whose support is $\mathbb{R}^n$) are equivalent to tempered fractional operators for a specific choice of operator parameters.

§1: Tempered Fractional Operators as a Special Case of Nonlocal Operators

In [3] we showed that through the introduction of the *equivalence kernel* the unweighted and weighted nonlocal operators presented in [4] are equivalent. In the following paragraph we briefly summarize this result. For $\boldsymbol{\alpha}:\mathbb{R}^n\times\mathbb{R}^n\to\mathbb{R}^n$ antisymmetric, $\mathbf{v}:\mathbb{R}^n\times\mathbb{R}^n\to\mathbb{R}^n$, and $u:\mathbb{R}^n\to\mathbb{R}$ the *nonlocal unweighted divergence and gradient* are defined as

(1) $$\mathcal{D}\mathbf{v}(\mathbf{x}) := \int_{\mathbb{R}^n}(\mathbf{v}(\mathbf{x},\mathbf{y})+\mathbf{v}(\mathbf{y},\mathbf{x}))\cdot\boldsymbol{\alpha}(\mathbf{x},\mathbf{y})d\mathbf{y}$$

(2) $$\mathcal{G}u(\mathbf{x},\mathbf{y}) := (u(\mathbf{y})-u(\mathbf{x}))\boldsymbol{\alpha}(\mathbf{x},\mathbf{y}).$$

Then, the nonlocal unweighted Laplacian is obtained by composing the divergence and gradient operators. For $\gamma=\boldsymbol{\alpha}\cdot\boldsymbol{\alpha}$ the *nonlocal unweighted Laplacian* is defined as

(3) $$\mathcal{L}=\mathcal{D}\mathcal{G}u(\mathbf{x}) = 2\int_{\mathbb{R}^n}(u(\mathbf{y})-u(\mathbf{x}))\gamma(\mathbf{x},\mathbf{y})d\mathbf{y}.$$

By introducing a two-point weight function $\omega : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$, we can define the *weighted nonlocal divergence and gradient* as

$$\mathcal{D}_\omega \mathbf{v}(\mathbf{x}) := \mathcal{D}(\omega(\mathbf{x},\mathbf{y})\mathbf{v}(\mathbf{x})) = \int_{\mathbb{R}^n} (\omega(\mathbf{x},\mathbf{y})\mathbf{v}(\mathbf{x}) + \omega(\mathbf{y},\mathbf{x})\mathbf{v}(\mathbf{y})) \cdot \boldsymbol{\alpha}(\mathbf{x},\mathbf{y})d\mathbf{y} \tag{4}$$

$$\mathcal{G}_\omega u(\mathbf{x}) := \int_{\mathbb{R}^n} \mathcal{G}u(\mathbf{x},\mathbf{y})\omega(\mathbf{x},\mathbf{y})d\mathbf{y} = \int_{\mathbb{R}^n} (u(\mathbf{y}) - u(\mathbf{x}))\boldsymbol{\alpha}(\mathbf{x},\mathbf{y})\omega(\mathbf{x},\mathbf{y})d\mathbf{y}. \tag{5}$$

Again, the weighted nonlocal divergence and gradient can be combined to obtain a *nonlocal weighted Laplacian*

$$\mathcal{L}_\omega u(\mathbf{x}) = \mathcal{D}_\omega \mathcal{G}_\omega u(\mathbf{x}) \tag{6}$$

$$= \int_{\mathbb{R}^n} \left[\int_{\mathbb{R}^n} (u(\mathbf{z}) - u(\mathbf{x}))\boldsymbol{\alpha}(\mathbf{x},\mathbf{z})\omega(\mathbf{x},\mathbf{z})d\mathbf{z} \right. \tag{7}$$

$$\left. + \int_{\mathbb{R}^n} (u(\mathbf{z}) - u(\mathbf{y}))\boldsymbol{\alpha}(\mathbf{y},\mathbf{z})\omega(\mathbf{y},\mathbf{z})d\mathbf{z} \right] \cdot \boldsymbol{\alpha}(\mathbf{x},\mathbf{y})\omega(\mathbf{x},\mathbf{y})d\mathbf{y}. \tag{8}$$

In [3] we proved that the unweighted and weighted Laplacian are equivalent with the choice of kernel

$$2\gamma_{eq}(\mathbf{x},\mathbf{y}) = \int_{\mathbb{R}^n} [\boldsymbol{\alpha}(\mathbf{x},\mathbf{y})\omega(\mathbf{x},\mathbf{y}) \cdot \boldsymbol{\alpha}(\mathbf{x},\mathbf{z})\omega(\mathbf{x},\mathbf{z}) \tag{9}$$

$$+ \boldsymbol{\alpha}(\mathbf{z},\mathbf{y})\omega(\mathbf{z},\mathbf{y}) \cdot \boldsymbol{\alpha}(\mathbf{x},\mathbf{y})\omega(\mathbf{x},\mathbf{y}) + \boldsymbol{\alpha}(\mathbf{z},\mathbf{y})\omega(\mathbf{z},\mathbf{y}) \cdot \omega(\mathbf{x},\mathbf{z})]d\mathbf{z} \tag{10}$$

used in the unweighted nonlocal Laplacian; that is, $\mathcal{L} = \mathcal{L}_\omega$ when $\gamma = \gamma_{eq}$. We utilize this equivalence kernel in the following analysis of the tempered fractional Laplacian.

The *tempered fractional Laplacian* is defined by

$$\mathcal{L}_{tem}\mathbf{u}(\mathbf{x}) := \int_{\mathbb{R}^n} (\mathbf{u}(\mathbf{y}) - \mathbf{u}(\mathbf{x})) \frac{e^{-\lambda|\mathbf{x}-\mathbf{y}|}}{|\mathbf{x}-\mathbf{y}|^{n+2s}} d\mathbf{y} \tag{11}$$

for $\lambda > 0$ and $0 < s < 1$. To show that the tempered fractional models are a special instance of the equivalence kernel, we made the choices

$$\omega(\mathbf{x},\mathbf{y}) = |\mathbf{y}-\mathbf{x}|\phi(|\mathbf{y}-\mathbf{x}|) \text{ with } \phi(|\mathbf{y}-\mathbf{x}|) = \frac{e^{-\lambda|\mathbf{x}-\mathbf{y}|}}{|\mathbf{y}-\mathbf{x}|^{n+1+s}} \tag{12}$$

$$\boldsymbol{\alpha}(\mathbf{x},\mathbf{y}) = \frac{\mathbf{y}-\mathbf{x}}{|\mathbf{y}-\mathbf{x}|}.$$

In [3] we see that when the above $\boldsymbol{\alpha}$ and ω are plugged into the equivalence kernel it results in a kernel of the form

$$\gamma_{eq}(\mathbf{x},\mathbf{y}) = \frac{F(n,s,\lambda,|\mathbf{x}-\mathbf{y}|)}{|\mathbf{x}-\mathbf{y}|^{n+2s}}. \tag{13}$$

One of the main contributions of this work is the following inequality, which we proved theoretically in one dimension and illustrated numerically.

$$\underline{C}e^{-\lambda|\mathbf{x}-\mathbf{y}|} \le F(n,s,\lambda,|\mathbf{x}-\mathbf{y}|) \le \overline{C}e^{-\lambda|\mathbf{x}-\mathbf{y}|}. \tag{14}$$

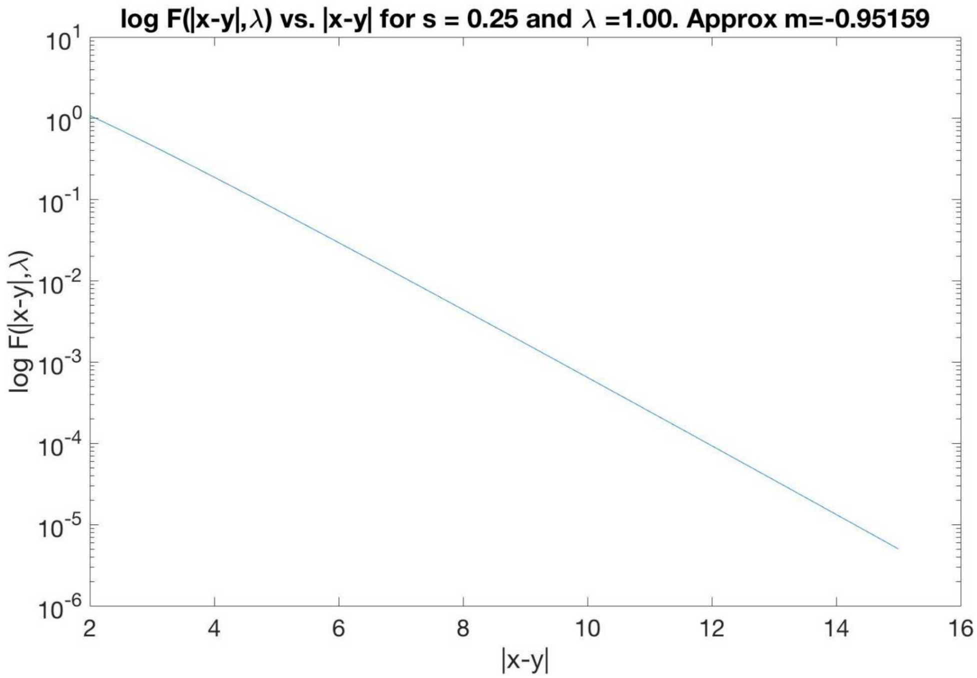
This inequality implies that the equivalence kernel associated with the choice of ω and $\boldsymbol{\alpha}$ in (12) asymptotically behaves like a tempered fractional kernel. Numerical tests conducted in MATLAB illustrate the behavior of F in (13). As indicated by the semilog plot in Figure 2, the function F exhibits the expected negative exponential behavior.

§2: Equivalence of the Tempered and Truncated Fractional Operators

In the second part of the project we want to show the tempered fractional operator is equivalent to the *truncated fractional Laplacian* defined

$$\mathcal{L}_{tr}\mathbf{u}(\mathbf{x}) := \int_{\mathbb{R}^n} (\mathbf{u}(\mathbf{y})-\mathbf{u}(\mathbf{x}))\frac{\mathbb{1}\{|\mathbf{x}-\mathbf{y}|<\delta\}}{|\mathbf{x}-\mathbf{y}|^{n+2s}}d\mathbf{y} \tag{15}$$

Figure 2. Example of a semilog plot of F vs. $|\mathbf{x}-\mathbf{y}|$ for the choices $\lambda = 1$ and $s = 0.25$. The linear behavior of the semilog plot indicates that F likely demonstrates the expected behavior.



for $0 < s < 1$ and some $\delta > 0$. One part of this is showing that the energies of the two operators are equivalent. Nonlocal operators have energies

$$E_i = \iint_{(\mathbb{R}^n)^2} (u(\mathbf{x}) - u(\mathbf{y}))^2 \gamma_i(\mathbf{x}, \mathbf{y}) d\mathbf{y} d\mathbf{x}. \tag{16}$$

For the fractional tempered and truncated operators, we have

$$\gamma_{tem} = \frac{e^{-\lambda|\mathbf{x}-\mathbf{y}|}}{|\mathbf{x}-\mathbf{y}|^{n+2s}} \qquad \gamma_{tr} = \frac{\chi\{|\mathbf{x}-\mathbf{y}| < \delta\}}{|\mathbf{x}-\mathbf{y}|^{n+2s}}. \tag{17}$$

So far, we showed that the truncated energy is bounded above by the tempered energy. In particular, $E_{tr} \leq e^{\lambda\delta} E_{tem}$. Our next step is to show that $E_{tem} \leq C(\lambda, \delta) E_{tr}$.

A future part of the project is showing that the two operators are equivalent by comparing their Fourier symbols.

Contributions Made to the Research Project

One of my major personal contributions was generating MATLAB scripts which could be used to visualize the operators and kernels of interest throughout the internship. Having a visual on these functions gave my research group insight into behaviors – both by confirming expected behaviors and by revealing unexpected behaviors, which are not reported in the current document. Another contribution was concocting a proof for one half of the energy equivalence: the truncated energy being bounded by the tempered energy. Additionally, I was involved in weekly meetings where my group discussed our recent progress and collaborate on ideas for moving forward with the research.

During the internship, I presented initial findings in the 2020 Sandia Poster Blitz. This was a digital poster session open to all of the summer interns at Sandia National Labs. Additionally, my research group and I are working on a research article to submit to the 2020 Sandia Summer Proceedings, which is scheduled to be published by the end of the year.

What new skills and knowledge did you gain?

I have gained a lot of knowledge both about my specific area of research and about adjacent topics. Throughout my work and research meetings with my peers, I've expanded upon the basis of knowledge I had about nonlocal vector calculus – my area of research. Additionally, the hosting facility provided me with access to multiple seminar series and a reading group which had focuses in related fields such as machine learning, physics informed neural networks, and more.

This internship also gave me the opportunity to work on my Matlab skills. I had used it before for some brief academic exercises. However, this internship pushed me to adapt and expand those skills to be useful in a work environment.

Research Experience Impact on My Academic/Career Planning

This internship has also impacted my thoughts about my future career path. Throughout my graduate career, I have spent a lot of time with fellow academics – my instructors and peers are all a part of academia. This internship provides the opportunity to meet people of similar educational levels that opted to follow a non-academic career path. It also gives me insight into what working a non-academic career could look like in the future. Previously, I was apprehensive about following a non-academic path because academia is what I'm most familiar with. However, I'm now quite interested in pursuing a non-academic career once I've completed my degree.

Relevance to the mission of NSF

This research project is part of a bigger effort whose main goal is to provide better predictive simulations for applications that can be described by nonlocal models. The latter provide an improved predictive capability for settings where traditional partial differential equations (PDEs) fail to describe the phenomenon at hand. This happens in particular in presence of multiscale or anomalous behavior; as an example, the fractional models mentioned in this report are able to catch anomalous diffusion which appears in subsurface transport applications and that cannot be described by standard PDEs. The analysis and simulation of diffusion or transport processes in the subsurface is extremely valuable for both the laboratory and for the NSF as it can be used to model, e.g., pollutant transport for nuclear waste disposal. However, the use of nonlocal and fractional models goes way beyond geoscience and includes mission applications that became extremely important during the past few months due to the COVID-19 outbreak. In fact, fractional models have been successfully used in the past to model the way viruses, like Ebola, spread (see, e.g. [1]).

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