Reconstructing the diffusion coefficient in fractional diffusion equations

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Abstract. We consider the inverse problem of identifying the diffusion coefficient in a time-fractional diffusion equation from noisy interior measurements of the density. To overcome the instability issue of the problem, we employ a mollification based technique to smooth out the noisy data. We derive consistency and stability results, and provide numerical examples to show the feasibility of the proposed approach.

Keywords: inverse problems, coefficient identification, fractional diffusion.

1. Introduction

Fractional partial differential equations are extensions of the classical models for which the usual derivatives are replaced by fractional-order ones. In the past few decades, such equations have gained increasing currency due to a promising wide range of applications in physics, geophysics, polymer sciences, and other areas; see for example [27, 11, 15] and the references therein.

This article is devoted to the problem of identifying (reconstructing) the variable parameter q in the time-fractional diffusion equation

$$\frac{\partial^\alpha u}{\partial t^\alpha}(x,t) = \frac{\partial}{\partial x}\left(q(x,t)\frac{\partial u}{\partial x}(x,t)\right) + f(x,t), \quad (x,t) \in (0,1)^2, \tag{1}$$

where the time-fractional derivative is taken in the Caputo sense. We shall assume $\alpha \in (0,1)$, and we further impose the boundary condition

$$q(0,t)\frac{\partial u}{\partial x}(0,t) = g(t). \tag{2}$$

More precisely, we study the following *inverse problem*: assume that q and u are related by equations (1)–(2), estimate $q|_\Omega$ from a noisy (and probably discrete) measurement u^ϵ of u, where Ω is some suitable compact subset of $[0,1]^2$.

In many scientific application the data u^ϵ can be acquired easily using nondestructive, and in many cases, noninvasive, procedures such as the Infrared Thermography. However, measuring the parameter q (characterizing the material properties of the hosting medium) would inevitably require a direct access and cannot be done remotely or nondestructively. For these reasons, this inverse problem is very important and can be used in various environmental, physical, or engineering applications.

Equation (1), and its variations, are found to be adequate models to describe anomalous diffusion, such as the sub-diffusion, which have been observed, for example, in transport processes in porous media, protein diffusion within cells, transport of ions in column experiments, movement of a material along fractals, etc.; see [30, 23, 8, 14, 12] for derivation and more concrete examples. For the analytical and numerical aspects of fractional-differential equations, the reader may consult [27, 11, 26, 1, 16, 22].

Inverse problems involving classical differential equations have been fairly examined in the past few decades. However, only a humble number publications treating fractional inverse problems have been established in spite of its significance in a variety of scientific and engineering applications. We mention some of the recent inverse problems involving fractional differential equations. Wang and Liu [32] considered the inverse problem of the determination of the initial distribution from internal measurements of $u(\cdot, T)$, their problem is in 2D and they used total variation regularization to obtain stable approximations of the backward problem. In [10], Deng and Yang proposed a numerical method based on the idea of reproducing kernel approximation to reconstruct the unknown initial heat distribution from a finite set of scattered measurements of transient temperature at a fixed final time. Zhang and Xu [34] considered the problem of identifying the time-independent source term f from the additional boundary data $u(0,\cdot)$. In [20], LI and GUO considered the identification of the diffusion coefficient and the order of the fractional derivative from the boundary data $u(0,\cdot)$. A tutorial on inverse problems for anomalous diffusion equations is given by Jin and Rundell [18]. The article summarizes some recent results and sheds the light on several open problems on the subject. See also [33, 21, 31, 17, 2, 3, 4] for other related inverse problems.

The aforementioned inverse problem is ill-posed; clearly if $\partial_x u$ vanishes on some open subset of Ω, then (1) provides no information about the parameter on that set, and hence no uniqueness. Moreover, the need to differentiate the (noisy) data makes the inverse solution instable with respect to perturbation in the data. To retain stability, we employ the regularization by mollification technique which has been introduced in [24, 25]. This amounts to computing the coefficient in (1)–(2) with u replaced by a (smoothed) mollified version of the data u^ϵ. In section 3, we prove consistency and stability theorems and give error bounds for the proposed method.

The rest of this paper is organized as follows. In Section 2 we present some definitions and lay the theoretical background, in Section 3 we prove the main results, numerical examples are contained in Section 4.

2. Preliminaries

In this section we collect some definitions and preliminary results pertaining to this work. We use the notation $\|f\|_K$ to denote the maximum norm of f over the set K, $C^n(K)$ to denote the space of n-times continuously differentiable functions, and $L^1(K)$ for the space of Lebesgue integrable functions over K.

2.1 Fractional calculus

Fractional calculus is a generalization of ordinary differentiation and integration to arbitrary non-integer order. It can be traced back to the year 1695 in a letter from Marquis de L'Hôpital to Gottfried Wilhelm Leibniz asking of the meaning of $d^n y/dx^n$ with $n = 1/2$. Since then several definitions have been given trying to accommodate the meaning of non-integer order derivatives and integrals.

To date, however, there is no unified definition of fractional derivative, but there are some accepted and common definitions in the literature. These definitions include but not limited to the Riemann-Liouville, Caputo, and Gränwald Letnikov definitions [27, 19]. Recently new definitions of fractional derivatives with applications to real world problems have emerged. In [7], Atangana and Baleanu introduced a new fractional derivative definition based on the generalized Mittag-Leffler function. Caputo and Fabrizio [9] presented a new definition of fractional derivative with a smooth kernel based on the exponential function. Comparison between various types of fractional derivatives applied to the fractional Allen Cahn and Freedman models can be found in [6, 13]. Saad et al. [29] used the optimal q-HAM analysis method to solve the fractional gas dynamics equation. An extension of the standard model of cubic isothermal auto-catalytic chemical system to the fractional case along with their numerical solutions using the q-homotopy analysis transform method is considered in [28]. See also the work by Al-Jamel et al. [5] were they studied the forced damped harmonic oscillator within the context of memory-dependent fractional derivative.

Contrary to the Riemann-Liouville definition, Caputo's definition of fractional derivative appears more frequently in the contexts of mathematical physics since it allows traditional (non-fractional) initial and boundary conditions to be incorporated in the mathematical model [27]. Therefore, in our model given by equation (1), we use the Caputo fractional derivative given by the following definition.

Definition 2.1. *The Caputo fractional derivative of order* $\alpha \in (0,1)$ *of a function* f *is defined by*

$$D^\alpha f(t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-s)^{-\alpha} f'(s) ds, \quad t > 0.$$

This definition can be adopted for functions of several variables as well. For instance, we define

$$\frac{\partial^\alpha f}{\partial t^\alpha}(x,t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-s)^{-\alpha} \frac{\partial f}{\partial t}(x,s) ds,$$

and similarly for the fractional derivative of f with respect to the spatial variable x. More about the properties and applications of Caputo derivatives can be found in [27, 19].

2.2 Mollification

We shall need the following definitions and results in the sequel. For more details, readers may consult the textbook [24].

Definition 2.2. *The* δ*-mollifier, denoted by* ρ_δ*, is defined by*

$$\rho_\delta(x) = \frac{1}{A\delta} \begin{cases} \exp\left(-x^2/\delta^2\right), & |x| \le 3\delta, \\ 0, & |x| > 3\delta. \end{cases}$$

where $A = \int_{-3}^{3} \exp(-s^2)\, ds$.

Definition 2.3. *The* δ*-mollification of* $f \in L^1(I)$ *on* K_δ*, denoted by* $J_\delta f$*, is defined by*

$$(J_\delta f)(x) = \int_{-3\delta}^{3\delta} \rho_\delta(s) f(x-s) ds = \int_{x-3\delta}^{x+3\delta} \rho_\delta(x-s) f(s) ds, \quad x \in K_\delta,$$

where $I = [0,1]$ *and* $K_\delta = [3\delta, 1-3\delta]$.

Let K be any compact subset of K_δ. Then we have the following auxiliary results [24].

Lemma 2.1. *If* $\|f''\|_I \le M$*, then*

$$\begin{aligned} \left\|(J_\delta f)' - f'\right\|_K &\le 3M\delta, \\ \|D^\alpha(J_\delta f) - D^\alpha f\|_K &\le \frac{3M}{\Gamma(2-\alpha)}\delta. \end{aligned}$$

Lemma 2.2. *Suppose that* $f, f^\epsilon \in C(I)$ *with* $\|f - f^\epsilon\|_I \le \epsilon$*. Then*

$$\begin{aligned} \left\|(J_\delta f)' - (J_\delta f^\epsilon)'\right\|_K &\le \frac{4}{A}\frac{\epsilon}{\delta}, \\ \|D^\alpha(J_\delta f) - D^\alpha(J_\delta f^\epsilon)\|_K &\le \frac{1}{\Gamma(2-\alpha)}\frac{4}{A}\frac{\epsilon}{\delta}. \end{aligned}$$

We conclude with the following corollary which we shall need in the sequel.

Corollary 2.1. *If $f \in C^1(I)$, then*

$$\min_K \{|f'(x)|\} \le \|(J_\delta f)'\|_K \le \|f'\|_I.$$

Proof. This follows from the fact that $(J_\delta f)'(x) = (J_\delta f')(x)$ and the mean-value theorem for integrals. □

3. Main results

We now prove stability, consistency, and convergence results for the mollification method. For convenience, we use the notations $J^\delta u(x,t)$ and $J_\delta u(x,t)$ to denote the δ-mollification with respect to the variables x and t, respectively.

Assume that $\Omega \subset K_\delta \times K_\delta$, and let q_δ and $q_{\delta,\epsilon}$ be the coefficients obtained by solving equations (1)–(2) when u is replaced by $J_\delta u$ and $J_\delta u^\epsilon$, respectively, then we have the following consistency and stability results:

Lemma 3.1. *If $f, g \in C(I)$, $\max\{\|\partial_{xx} u\|_I, \|\partial_{tt} u\|_I\} \le U < \infty$, and $\min_\Omega |\partial_x u(x,t)| \ge R > 0$, then there exists a constant C independent of δ such that*

$$\|q - q_\delta\|_\Omega \le C\delta.$$

Proof. Set $E_\delta(x,t) = q(x,t) - q_\delta(x,t)$. Integrating both sides of (1) from 0 to x and using the boundary condition (2) yield

$$\begin{aligned}\partial_x u(x,t)\partial_x J^\delta u(x,t) E_\delta(x,t) &= \left(\int_0^x \left[\partial_t^\alpha u(s,t) - f(s,t)\right] ds + g(t)\right) \partial_x J^\delta u(x,t) \\ &\quad - \left(\int_0^x \left[\partial_t^\alpha J_\delta u(s,t) - f(s,t)\right] ds + g(t)\right) \partial_x u(x,t).\end{aligned}$$

Let $\widetilde{u}_\delta = J^\delta u - u$. Using Corollary 2.1, Lemma 2.1, and simple manipulation, for all (x,t) in Ω we have

$$\begin{aligned}R^2 |E_\delta(x,t)| &\le \left(\int_0^x \left[|f(s,t)| + |\partial_t^\alpha u(s,t)|\right] ds + |g(t)|\right) \|\partial_x \widetilde{u}_\delta\|_\Omega \\ &\quad + \int_0^x |\partial_t^\alpha J_\delta u(s,t) - \partial_t^\alpha u(s,t)|\, ds\, \|\partial_x u\|_\Omega \\ &\le 3U\delta \left(\|f\|_I + \frac{\|\partial_t u\|_I}{\Gamma(2-\alpha)} + \|g\|_\Omega\right) + \frac{3U\delta\, \|\partial_x u\|_\Omega}{\Gamma(2-\alpha)} \le C\delta,\end{aligned}$$

for some constant C independent of δ, which completes the proof. □

Lemma 3.2. *Suppose that f, g, and u satisfy the hypothesis of Lemma 3.1. If $\|u - u^\epsilon\|_I \le \epsilon$ and $2\epsilon < AR\delta$, then there exists a constant C independent of ϵ and δ such that*

$$\|q_\delta - q_{\delta,\epsilon}\|_\Omega \le C \frac{\epsilon}{RA\delta - 2\epsilon}.$$

Proof. Set $E_{\delta,\epsilon} = q_\delta - q_{\delta,\epsilon}$. Then from (1) and (2), for all $(x,t) \in \Omega$ we have

$$\left(\partial_x J^\delta u \cdot \partial_x J^\delta u^\epsilon \cdot E_{\delta,\epsilon}\right)(x,t) = \left(\int_0^x [f(s,t) - \partial_t^\alpha J_\delta u(s,t)]\, ds + g(t)\right) \partial_x J^\delta u^\epsilon$$
$$- \left(\int_0^x (f(s,t) - \partial_t^\alpha J_\delta u^\epsilon(s,t) ds + g(t)\right) \partial_x J^\delta u.$$

It follows from Lemma 2.2 and the reverse triangle inequality that

$$0 < R - \frac{2\epsilon}{A\delta} \leq \left|\partial_x J^\delta u^\epsilon(x,t)\right|$$

for all $(x,t) \in \Omega$, and so, with a little algebra, we have

$$\left(R^2 - \frac{2R\epsilon}{A\delta}\right) |E_{\delta,\epsilon}| \leq \int_0^x |\partial_t^\alpha J_\delta u^\epsilon(s,t) - \partial_t^\alpha J_\delta u(s,t)|\, ds \left|\partial_x J^\delta u(x,t)\right|$$
$$+ \left(\int_0^x [|f(s,t)| + |\partial_t^\alpha J_\delta u(s,t)|]\, ds + |g(t)|\right) \|\partial_x \widetilde{u}\|_\Omega,$$

where $\widetilde{u} = J^\delta(u^\epsilon - u)$. Thus, using Lemma 2.2 and Corollary 2.1 we obtain

$$\left(R^2 - \frac{2R\epsilon}{A\delta}\right) \|E_{\delta,\epsilon}\|_\Omega \leq \frac{2\epsilon}{A\delta}\left(\|f\|_I + \|g\|_\Omega + \frac{\|\partial_t u\|_I}{\Gamma(2-\alpha)}\right) + \frac{2\epsilon\|\partial_x u\|_I}{A\Gamma(2-\alpha)\delta} \leq C\frac{\epsilon}{\delta},$$

which ends the proof. □

From the triangle inequality, Lemma 3.1 and Lemma 3.2, we obtain the main convergence result.

Theorem 3.1. *Under the assumptions of Lemma 3.1 and Lemma 3.2, we have*

$$\|q - q_{\delta,\epsilon}\|_\Omega \leq C\left(\delta + \frac{\epsilon}{RA\delta - 2\epsilon}\right)$$

for some constant C independent of ϵ and δ.

Remark 3.1. If δ is chosen so that $\delta = O(\epsilon^\mu)$ for some $0 < \mu < 1$, then we obtain the convergence result

$$\|q - q_{\delta,\epsilon}\|_\Omega \to 0, \quad \text{as } \epsilon \to 0.$$

Moreover, taking $\mu = 1/2$, we have the optimal convergence rate

$$\|q - q_{\delta,\epsilon}\|_\Omega = O(\epsilon^{1/2}).$$

4. Numerical examples

In this section we demonstrate how to implement the proposed method in a practical algorithm and we present several numerical examples.

Upon integrating (1) and using the boundary condition (2), the approximate inverse solution can be written as

$$q_{\delta,\epsilon}(x,t) = \frac{\int_0^x \left[\partial_t^\alpha J_\delta u^\epsilon(s,t) - f(s,t)\right] ds + g(t)}{\partial_x J^\delta u^\epsilon(x,t)}. \tag{3}$$

In practice the measured data is discrete, and so, the right-hand side of (3) must be discretized. To this end, we approximate the integral using a composite trapezoidal rule, and the fractional derivative is approximated using the algorithm proposed in [25]. For the partial derivative in the denominator, we use the centered difference approximation.

For simplicity, the noisy data u^ϵ is computed according to the formula

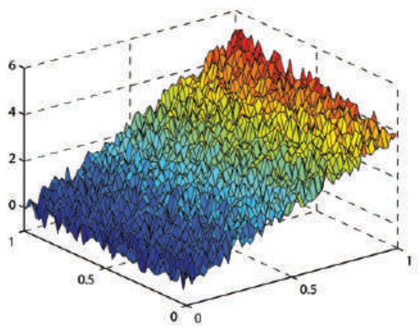
$$u^\epsilon(x_i,t_j) = u(x_i,t_j) + \epsilon\gamma_{i,j}, \quad i = 1,\ldots,N_x, \quad j = 1,\ldots,N_t,$$

where ϵ represents the noise level, and $\gamma_{i,j}$ is a uniformly distributed random number in $[-1,1]$. In the experiments below, we take $\Omega = [0,1]^2$ and we use uniform grid points with $N_x = N_t = 150$. The mollification parameter δ, representing the degree of smoothing, is determined by the Principle of Generalized Cross Validation as described in the article [24].

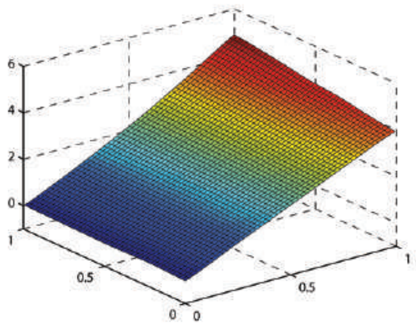
The error in the approximation is measured using the relative root-mean-square error which is defined as

$$\text{RMS} = \frac{\sqrt{\sum_{i=1}^{N_x}\sum_{j=1}^{N_t}\left[q(x_i,t_j) - q_{\delta,\epsilon}(x_i,t_j)\right]^2}}{\sqrt{\sum_{i=1}^{N_x}\sum_{j=1}^{N_t}\left[q(x_i,t_j)\right]^2}}.$$

We note that the RMS is just the discrete version of the relative L^2-error.



(a) Noisy data



(b) Smoothed data

Figure 1: Smoothing the data of Example 4.1.

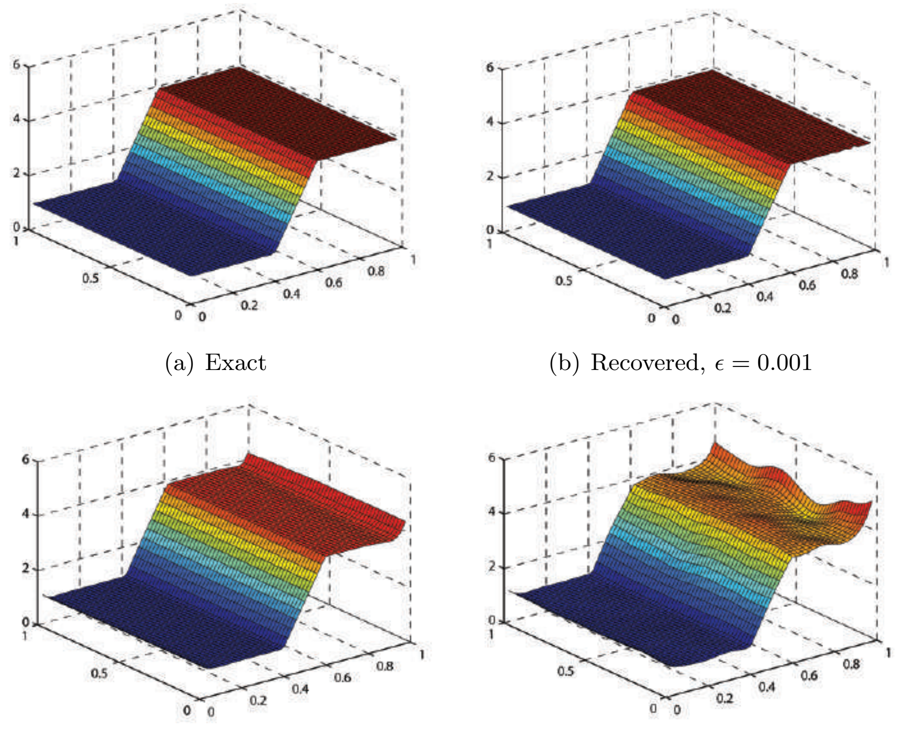
Table 1: Error results for Example 4.1 at several noise levels ϵ.

Noise Level	0.1%	1%	10%
(i) Raw	1.39E−2	1.41E−1	7.39E+1
(ii) Mollified	4.80E−3	3.56E−2	4.10E−2

Example 4.1. We consider equations (1)–(2) with $u(x,t) = tx^2 + 4x$ and $\alpha = 0.75$. The function f is chosen so that the exact diffusion coefficient is

$$q(x,t) = \begin{cases} 1, & 0 \le x \le 0.4, \\ 15x - 5, & 0.4 < x \le 0.6, \\ 4, & 0.6 < x \le 1. \end{cases}$$

The error results using the noisy (Raw) and smoothed (Mollified) data are presented in Table 1. Figure 1 shows the plots for the exact data, noisy data, and the denoised (smoothed) data when the noise level in the data is $\epsilon = 10\%$. The recovered parameter q at different noise levels are shown in Figure 2.



(a) Exact

(b) Recovered, $\epsilon = 0.001$

(c) Recovered, $\epsilon = 0.01$

(d) Recovered, $\epsilon = 0.1$

Figure 2: Exact and recovered parameter q in Example 4.1.

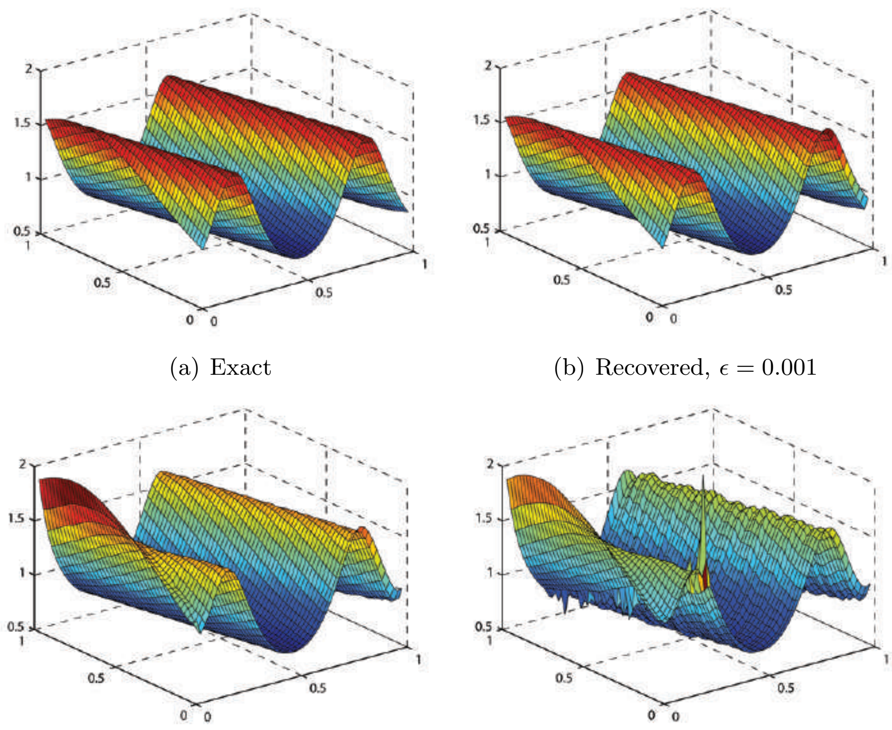
Example 4.2. In this experiment, we consider equations (1)–(2) with $\alpha = 0.5$ and $u(x,t) = 8x \exp(t) \operatorname{erfc}(\sqrt{t})$, where $\operatorname{erfc}(\cdot)$ is the complementary error function. The source term f is chosen so that the exact diffusion coefficient is

$$q(x,t) = (1 - 0.4\sin(10x + 2t))^{-1}.$$

The error results using the noisy and smoothed data are summarized in Table 2. Plots for the recovered parameter q at different noise levels are shown in Figure 3.

Table 2: Error results for Example 4.2 at several noise levels ϵ.

Noise Level	0.1%	1%	10%
(i) Raw	1.50E−2	1.57E−1	9.07E+2
(ii) Mollified	5.60E−3	3.67E−2	4.75E−2



(a) Exact (b) Recovered, $\epsilon = 0.001$

(c) Recovered, $\epsilon = 0.01$ (d) Recovered, $\epsilon = 0.1$

Figure 3: Exact and recovered parameter q in Example 4.2.

5. Conclusion

We considered mollification based technique to solve the inverse problem of identifying the diffusion coefficient in a one-dimensional time-fractional diffusion equation from noisy interior data. We proved consistency and convergence theorems for the proposed approach. Numerical examples are also given to elucidate and validate the proposed method. Numerical results show that this approach is powerful and indicate noteworthy results.

We observe from the numerical tests above that for small noise levels the mollification method gives slight improvement in the error. However for larger noise levels, the method shows noteworthy improvements over using directly the raw (non-smoothed) data. In the future, we hope to carry the analysis for the discretized problem, and generalize this approach to problems in higher spatial dimensions which is more relevant in scientific applications.

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