UNIVERSIDAD NACIONAL DE COLOMBIA

Ecuaciones Diferenciales Fraccionarias y Problemas Inversos

Fractional Differential Equations and Inverse Problems

Manuel D. Echeverry

Universidad Nacional de Colombia
Facultad de Ciencias, Área Curricular de Matemáticas
Medellín, Colombia
2020

Ecuaciones Diferenciales Fraccionarias y Problemas Inversos

Fractional Differential Equations and Inverse Problems

Manuel D. Echeverry

Tesis presentada como requisito parcial para optar al título de:
Doctor en Ciencias-Matemáticas

Director
Carlos E. Mejía Salazar

Línea de Investigación:
Análisis Numérico
Grupo de Investigación:
Computación Científica

Universidad Nacional de Colombia
Facultad de Ciencias, Área Curricular de Matemáticas
Medellín, Colombia
2020

A mi madre.

Agradecimientos

Durante todo el proceso de escritura de este trabajo han pasado muchas personas por mi vida, espero no olvidarme de ninguna en este aparte, pero no tengo más que buenas palabras y deseos para todos quienes hicieron parte de mis días en este camino.

Comenzaré por mencionar a mi madre, Mariela Echeverry, a quien además dedico todo este trabajo, el cual en parte también es suyo. El profesor Carlos E. Mejía es alguien a quien he admirado por largo tiempo y a quien estoy profundamente agradecido por todos los años que ha dedicado a enseñarme; también a mis profesores Margarita Toro, Jhon Jader Mira, Carlos Vélez y Juan Diego Vélez por su dedicada labor.

Agradezco especialmente a los jurados Adriano De Cezaro, Marcos A. Capistrán y Jorge Mauricio Ruíz Vera por tomarse el trabajo de revisar y de hacer sugerencias que mejoraron el resultado final. Este trabajo no hubiera sido posible sin la financiación de la convocatoria 647 de Colciencias.

A mi novia Nathalia García, que ha alegrado mis días.

Javier Verbel y Mauricio Cepeda fueron grandes compañeros de oficina, de estudio y de charlas, que muchas veces terminaban en Bantú. Tuvimos la suerte de compartir nuestros estudios con personajes muy afables, entre los cuales cuento a Gustavo Restrepo, Samir Posada, Sebastián Vélez y Juan Sebastián Jaramillo.

Muchos han sido los estudiantes que he tenido estos años, pero Los Babies cuentan con un lugar privilegiado. Daniel Sánchez, Kewin Evers, Andrés Felipe López, Carlos Acosta y Kevin Flórez, han pasado de ser jóvenes prometedores a hombres a quienes aprecio y admiro.

A mi familia, en especial a mi hermano y a mis primos Luisa, Ramiro y Erwin, que han estado ahí para mí desde que tengo memoria. También agradezco a Vitto y a La Bestia por su incondicional compañía todos estos años.

He tenido la suerte de contar con mis amigos Sebastián López, Sebastián Correa, Luis Carlos Aristizábal, Ángela María Pérez, Esperanza Marín, Andrés Giraldo, Jorge Sepúlveda, Jorge Londoño, Carolina Grajales y Andrés Buitrago. Espero poder seguir contando con su buena compañía.

También agradezco a Sandra Montoya por su impecable trabajo.

Por último quiero mencionar a quienes me acompañaron durante mi tiempo en Valencia, allí conocí a muchas personas, pero recuerdo con especial afecto a Sara Echeverri, Dominika Grobarčíková, Julian Martines Silva, Rodhlann O'Larcain, Luis Gracia y Joshua Nancarrow.

Agraïments

Amb les poques paraules que puc expressar en aquest llengua, vull dir als Professors Pep Mulet i Mestre i Antonio Baeza, de l'Universitat de València, que estic profundament agraït per tots les matins prenent cafè i les moltes coses que vaig aprendre d'ambdós. També vull dir-li a Iván Estipiná Martos que tinc molta sort de tenir un amic com tu. Me'n alegra haver pogut conèxer-los. Moltes gràcies.

Acknowledgment

I'll start with my mother, to whom this thesis is dedicated to. Professor Carlos E. Mejía is someone I have admired for long and to whom I am deeply grateful. I acknowledge to the juries of this thesis, Adriano De Cezaro, Jorge Mauricio Ruíz Vera and Marcos A. Capistrán, for their rigorous labour and for their interesting suggestions that improved the final result. This work was possible thanks to *convocatoria 674* of Colciencias.

Abstract

Our goal is the study of identification problems in the framework of transport equations with fractional derivatives. We consider time fractional diffusion equations and space fractional advection dispersion equations. The majority of inverse problems are ill-posed and require regularization. In this thesis we implement one and two dimensional discrete mollification as regularization procedures.
The main original results are located in chapters 4 and 5 but chapter 2 and the appendices contain other material studied for the thesis, including several original proofs.
The selected software tool is MATLAB and all the routines for numerical examples are original. Thus, the routines are part of the original results of the thesis.
Chapters 1, 2 and 3 are introductions to the thesis, inverse problems and fractional derivatives respectively. They are survey chapters written specifically for this thesis.

Keywords: Fractional Derivatives, Mollification, Inverse Problems, Differential Equations.

Resumen

Nuestro objetivo es el estudio de problemas de identificación en el marco de ecuaciones de transporte con derivadas fraccionarias. Consideramos ecuaciones difusivas con derivada temporal fraccionaria y ecuaciones de advección dispersión con derivada espacial fraccionaria. La mayoría de los problemas inversos son mal condicionados y requieren regularización. En esta tesis implementamos procedimientos de regularización basados en molificación discreta en una y dos dimensiones.
Los principales resultados originales se encuentran en los capítulos 4 y 5 pero el capítulo 2 y los apéndices contienen material adicional estudiado para la tesis incluídas varias demostraciones originales.
La herramienta de software escogida es MATLAB y todas las rutinas para los ejemplos numéricos son originales, de manera que las rutinas son parte de los resultados originales de la tesis.
Los capítulos 1, 2 y 3 son introductorios a la tesis, a los problemas inversos y a las derivadas fraccionarias respectivamente. Se trata de capítulos monográficos escritos especialmente para esta tesis.

Palabras clave: Derivadas Fraccionarias, Molificación, Problemas Inversos, Ecuaciones Diferenciales.

Contents

1. Introduction

In this thesis we consider some interactions between two current and challenging topics of applied mathematics: fractional differential equations and inverse problems. Both topics are known since long time ago but only recently, let's say since personal computers became widely available around 1985, research on both subjects show remarkable activity.
In this introduction we start with some historical notes and follow with short presentations of the results obtained in the Thesis.

1.1. Historical development

1.1.1. Fractional derivatives

Fractional derivatives are as old as derivatives of integer order and many remarkable mathematicians participate in the development of the concept. All began with a 1695 letter from Leibniz to L'Hospital, asking him about what happens in d^n/dx^n, if $n = 1/2$.
Some decades latter (1730) Riemann mentioned the same idea for any real number. Lagrange (1772) made advances in differential operators and Laplace (1812) provided some of the first formulae for fractional derivatives, for instance, he showed that the fractional derivative of function $y = x^m$ is

$$\frac{d^n y}{dx^n} = \frac{\Gamma(m-1)}{\Gamma(m-n+1)} x^{m-n}, \qquad m \geq n. \tag{1-1}$$

Some time later, a general approach was made, and the Riemann-Liouville fractional derivative was defined as

$${}_{RL}D_x^{\alpha} f(a) = \frac{d^m}{dx^m}\left[\frac{1}{\Gamma(m-\alpha)}\int_0^a \frac{f^{(m)}(\tau)}{(a-\tau)^{\alpha+1-m}}d\tau\right], m-1 < \alpha < m. \tag{1-2}$$

A drawback of this definition is that the derivative of a constant is not zero. Fortunately other definitions appear later on, for instance, the Caputo fractional derivative, for any α, given by

$$D_x^{\alpha} f(a) = \frac{1}{\Gamma(m-\alpha)}\int_0^a \frac{f^{(m)}(\tau)}{(a-\tau)^{\alpha+1-m}}d\tau. \tag{1-3}$$

where m is a positive integer and $f^{(m)}(\tau)$ is the standard derivative of order m in τ.

The first specialized conference on fractional calculus took place at the University of New Haven in West Haven, Connecticut, USA in 1974 and the first monograph in the field is Oldham and Spanier 1974 ([37]), published the same year. Other monographs worth mentioning are the books Miller and Ross 1993 [33] and Podlubny 1999 [38] and the papers Gorenflo and Mainardi 2008 [19], Sun et al. 2018 [46] and the specialized Benson, Meerschaert and Revielle 2013 [10].

1.1.2. Inverse problems

According to Groetsch, (Groetsch 1993 [20]) inverse problems are as old as the greek philosopher Plato, whose *Allegory of the cave* consists on reconstructing "reality" from observations of shadows cast upon a wall. The definition of an inverse problem is based on the definition of other problem, the so called *direct* problem. Thus, most of the time, we consider particular instances of inverse problems rather than considering them in general.
In the beginning of the twentieth century, the french mathematician Jacques Hadamard established the three defining conditions for a *well-posed* problem: Existence of a solution, uniqueness of the solution and stability of the solution. Problems that do not satisfy at least one of the three conditions are called *ill-posed* problems.
In general, inverse problems are ill-posed in the sense of Hadamard, that is:

1. They may not have a solution.

2. They may have more than one solution.

3. The solution is not continuous with respect to perturbations in the data.

In order to numerically solve an inverse problem, there are two main factors:

1. A direct problem solver: Very often the solution of the inverse problem is based on an iterative procedure that in each step requires the solution of the direct problem.

2. A regularization method: The objective is to recover stability with respect to perturbations in the data. The idea is to solve a different but stable problem whose solution approximates the solution of the original problem. The construction of the stable problem is known as regularization.

Among the monographs on inverse problems, we mention Groetsch 1993 [20], Murio 1993 [34], Hansen 2010 [22] and Hansen 1998 [21].
Among the available regularization methods, the more common is Tikhonov regularization ([20, 21]) and the selected regularization procedure for this thesis is the mollification method ([6, 34]).
In this thesis we develop new methodology for multidimensional discrete mollification. It resembles Acosta and Burger 2012 [5] but we provide a new insight and more details.

1.2. Motivation

Inverse problems arise in several branches of engineering, environmental sciences and other subjects. When based on differential equations, they are basically of two types:

1. The direct problem requires boundary data. If some part of the boundary data is missing, an inverse problem arises. In order to solve it, some overposed data on the rest of the boundary is required.

   Example Mejía Piedrahita 2017 [31] The direct problem is

   $$\begin{aligned} D_t^{(\alpha)} u + a u_x &= d u_{xx}, \quad x > 0, \quad t > 0, \\ u(x,0) &= 0, \quad x > 0, \\ u(0,t) &= \rho(t), \quad t \geq 0, \quad u(x,t) \text{ bounded as } x \to \infty, \end{aligned} \tag{1-4}$$

   where u is the solute concentration, u_x is the dispersion flux, the constants $a > 0$, $d > 0$ represent the average fluid velocity and the dispersion coefficient, respectively, and $D_t^{(\alpha)} u$ denotes the Caputo fractional derivative of order $\alpha, 0 < \alpha < 1$.

   The time fractional inverse advection-dispersion problem (TFIADP) is

   $$\begin{aligned} D_t^{(\alpha)} u(x,t) + a u_x(x,t) &= d u_{xx}(x,t), \quad x > 0, \quad t > 0, \\ u(1,t) &= \rho(t), \quad t > 0, \quad \text{data}, \\ u_x(1,t) &= \sigma(t), \quad t > 0, \quad \text{data}, \\ u(0,t) &= \xi(t), \quad t \geq 0, \quad \text{unknown}, \\ u_x(0,t) &= \beta(t), \quad t \geq 0, \quad \text{unknown}, \\ u(x,0) &= 0, \quad x > 0. \end{aligned} \tag{1-5}$$

   The distributed interior data functions ρ and σ are not known exactly. Moreover, their measured approximations ρ^ε and σ^ε satisfy the estimates $\|\rho - \sigma^\varepsilon\|_\infty < \varepsilon$ and $\|\rho - \sigma^\varepsilon\|_\infty < \varepsilon$ for a prescribed maximum level of noise in the data $\varepsilon > 0$. For the examples is added noise with normal distribution.

   The numerical identification process of ξ and β is based on the overdetermined interior data ρ^ε and σ^ε.

2. The direct problem requires the knowledge of all coefficients and forcing terms in the equation. If some of them are missing, there is an inverse problem. In this case, the overposed data is generally of two types: The solution of the differential equation is known at a particular point of the domain for all times or a final time distribution of

the solution is known.

This thesis deals with inverse problems of this type. There are identifications of forcing term factors and other parameter estimation problems.

The time fractional differential operators are operators with memory and the space fractional differential operators are nonlocal operators. Some models of science and engineering require the combination of both, that is, time and space fractional differential operators.
Of paramount importance is the modeling of *anomalous diffusion* [17] in porous media by fractional differential equations.
We deal with function or parameter identification inverse problems in the framework of time fractional and space fractional differential equations. The associated direct problems are based on diffusion equations or advection-dispersion equations. The solved inverse problems are potentially useful in particular instances of flow in porous media.

1.3. The interactions

1.3.1. Time fractional differential equations

Time fractional differential equations are models for a variety of situations in engineering and sciences ([27, 53]). Based on time fractional differential equations (tFDE), there are ill-posed problems, namely, the problems investigated in [31, 50] and there are well-posed problems, for instance [13].
Our concern is a time fractional diffusion equation. More precisely, we are interested in an initial/boundary value problem, in which the time derivative is a Caputo fractional derivative of order $\alpha,\ 0<\alpha<1$.
We are interested in the following initial/boundary value problem:

$$\left.\begin{array}{llll} D_t^{\alpha}u(z,t)-(Lu)(z,t) & = p(t)f(z), & z\in\Omega & t\in(0,T) \\ u(z,t) & =0, & z\in\partial\Omega & t\in(0,T) \\ u(z,0) & =0, & z\in\bar{\Omega} & \end{array}\right\} \tag{1-6}$$

where $\Omega\subset\mathbb{R}^d$ and:

$$Lu(z) \;=\; \sum_{i=1}^{d}\frac{\partial}{\partial z_i}\left(\sum_{j=1}^{d}a_{ij}(z)\frac{\partial}{\partial z_j}u(z)\right)+c(z)u(z), z\in\Omega. \tag{1-7}$$

If we think of this problem as the model for a contaminant diffusion in groundwater, then $f(z)$ plays the role of contaminant discharge intensity and $p(t)$ is an attenuation coefficient. In this thesis we implement the regularization method known as discrete mollification to solve the following inverse problems:

1. Identification of the unknown source factor $f(z)$ in Equation (1-6) based on the overposed data $u(z,T) = q(z)$. Time T is a final time and the data $q(t)$ are not known exactly; what is known is a measurement q^ϵ so that $\|q - q^\epsilon\|_\infty < \epsilon$.

2. Identification of the unknown time dependent factor $p(t)$ of the forcing term in equation (1-6) based on the overposed data given by a complete history of u at a specific point of the domain.

1.3.2. Space fractional differential equations

There are many applications of space fractional differential equations in science and engineering ([11, 17]) and generally correspond to the modeling of anomalous diffusion in porous media.

Based on space fractional differential equations, there are parameter estimation problems that are well-posed, namely [7, 23] and there are other estimation problems that are numerically solved by a history matching method combined with Tikhonov regularization. Among them, we mention [48] and [52].

We are interested in several simultaneous coefficient identification problems based on the following direct problem related to the tracing of a non reactive contaminant in groundwater:

$$\frac{\partial C}{\partial t} = -v\frac{\partial C}{\partial x} + D\frac{\partial^\alpha C}{\partial x^\alpha} + f(x,t) \tag{1-8}$$

Here C is the solute concentration, v is the pore-water velocity, D is the dispersion coefficient, $0 < t$, $x \in [0, L]$, $\frac{\partial^\alpha C}{\partial x^\alpha}$ is the Caputo fractional derivative of the concentration C of order α with $1 < \alpha \leq 2$ and $f(x,t)$ is a forcing term.

Together with equation (5-1) there are an initial condition and a set of boundary conditions. Examples of them are (see [48]):

$$C(x,0) = 0 \quad \text{initial condition} \tag{1-9}$$

$$C(0,t) = C_0 \; \text{left boundary condition, Dirichlet type} \tag{1-10}$$

$$\frac{\partial C}{\partial x}|_{x=L} = 0 \quad \text{right boundary condition, Neumann type} \tag{1-11}$$

The direct problem consists on finding C that satisfies (5-1)-(5-4) assuming all parameters are known.

We solve several coefficient identification problems based on two kinds of overposed data: A complete history of the concentration at a specific point of the domain or a final time distribution of the concentration.

1.4. The contents

The rest of the thesis is organized as follows:

Chapter 2 is an introduction to inverse problems and the regularization method known as discrete mollification. Fractional derivatives are introduced in chapter 3. This chapter contains several definitions of fractional derivatives but the problems solved in this thesis are based on Caputo fractional derivatives. The two inverse problems related to time fractional differential equations are presented in chapter 4 and chapter 5 deals with the inverse problems associated to space fractional differential equations. The conclusions and final remarks are in chapter 6 and there is an appendix which contains some other related material.

Contributions of this Thesis

This thesis has original review sections on inverse problems, fractional calculus and 2D discrete mollification. The 2D mollification operator was introduced by Acosta and Bürger in [5] but they do not consider enough details. This thesis contains a detailed description of this operator and it includes several original proofs.
Our original work on space dependent source term identification, the subject of section 4.2, was published in [16].
The results on time dependent source term identification included in section 4.3 are original. On this subject, we have further work in a preprint whose title is *Identification of a time-dependent source factor for a time-fractional diffusion equation.*
Our work on parameter estimation in the framework of space fractional advection dispersion equations, the subject of Chapter 5, is contained in a work in progress whose title is *Efficient parameter estimation in a solute transport model.*
Our MATLAB routines are original but they include calls to mollification routines prepared by C.D. Acosta.

2. Inverse Problems and Discrete Mollification

2.1. Inverse Problems

When the orbit of Uranus was observed, it seemed to be anomalous considering the Laws for the stellar motions. Then, independently and almost at the same time, Adams and Le Verrier, as is mentioned in [9, pp. 373, 401], trying to explain the discrepancies in the transit, and considering the Newton's Laws, established the necessity of the existence of another planet passing nearly the first one. They did not just predicted the presence of the celestial body, moreover, they calculated the circuit of it. And, as it is mentioned in [20], basically, they solved an inverse problem, in the sense that they found the *cause* given the *effect*, considering the Laws of Newton as the right model for the behavior of satellites. Soon after the considerations made by them, the new planet was found and was given the name of Neptune. This fact was fascinating and motivates some considerations that will be discussed bellow.
The general framework is illustrated in figure **2-1**

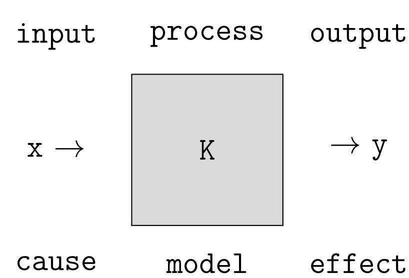

Figure 2-1.:

We are interested in the problem concerning the search for the *process* from *output* and *input*, or, what is more often wanted, the *input* from the *output* and the *process*. These problems are called inverse and the methods involving the search of their solutions, will be the core of the following study.
Hadamard, in the beginning of the century, established the idea of *well-posed* problems by the following conditions:

- Existence: there exists a solution for the problem.
- Uniqueness: that solution has to be unique.
- Continuity: the solution depends continuously on the data.

If at least one of the conditions is not satisfied, the problem is called *ill-posed*. Hadamard though that any problem that is *ill-posed* does not come from a rightly well formulated physical question. Later, that proved to be false since many ill-posed problems come from applications.
As an example of an inverse problem, we exhibit a linear system of equations $Ax = b$, in which the requesting datum is x since A and b are known. Depending on the properties of the matrix, the problem will be *ill-posed*. Illustrating this, consider the system

$$\begin{pmatrix} 1 & 1 \\ 1.0001 & 1 \end{pmatrix} x = \begin{pmatrix} 0 \\ 0.0001 \end{pmatrix} \tag{2-1}$$

$$Ax = b, \tag{2-2}$$

The solution is $x = (-1, 1)^\intercal$, but if the vector $(0, 0.0001)^\intercal$ is changed to $(0, 0)^\intercal$, then the solution will be $(0, 0)^\intercal$, which is highly different to the original one. Then, for a little noise, this problem carries big changes in the solution.

Not all inverse problems come from linear algebra, some very interesting ones are posed in the way

$$\int_\Omega input \times system \; d\Omega = output, \tag{2-3}$$

which can be seen as a direct problem if the output is computed from the input, but in some cases, the input is the target. One notable ill-posed problem to be addressed in this way, is a Fredholm integral equation of the first kind with a square integrable kernel [26], which can be written as follow

$$\int_0^1 K(s,t) f(t) dt = g(s), \qquad 0 \le s \le 1, \tag{2-4}$$

where the functions K and g are known, and f is the unknown. This task happens to be full of issues, because this kind of equations do not satisfy any of the Hadamard conditions of well-posing. This is addressed in [20], from where it is taken the next example to illustrate the ill-posedness that these problems could exhibit. If g satisfies

$$g(s) = \int_0^1 K(s,t) f(t) dt, \tag{2-5}$$

with

$$K(s,t) = \begin{cases} t(1-s), & 0 \le t \le s, \\ s(1-t), & s \le t \le 1, \end{cases} \tag{2-6}$$

then, it can be shown that g is the solution of the boundary value problem

$$g''(s) + f(s) = 0, \qquad 0 < s < 1 \tag{2-7}$$
$$g(0) = g(1) = 0. \tag{2-8}$$

Now, taking $g_\epsilon(s) = \epsilon(s-1)sin(s/\epsilon)$, for $\epsilon \ll 1$, function f takes the form

$$f(s) = 2cos\left(\frac{s}{\epsilon}\right) - \frac{(1-s)}{\epsilon}sin\left(\frac{s}{\epsilon}\right) \tag{2-9}$$

which experiences a large perturbation.
When kernel K is square integrable, i.e.

$$\|K\|_2^2 := \int_0^1 \int_0^1 K(s,t)^2 dsdt < \infty, \tag{2-10}$$

then

$$K(s,t) = \sum_{i=1}^{\infty} \mu_i u_i(s) v_i(t). \tag{2-11}$$

The functions u_i and v_i are called the *singular functions* of K, and the numbers μ_i are the *singular values* of it. These functions are orthonormal with respect the inner product $\langle\cdot,\cdot\rangle$ defined by

$$\langle \phi, \psi \rangle = \int_0^1 \phi(t)\psi(t)dt \tag{2-12}$$

The singular values of K are nonnegative and satisfy $\sum_{i=1}^{\infty} \mu_i^2 = \|K\|_2^2$.
Now, returning to the Fredholm equation, we obtain

$$\sum_{i=1}^{\infty} \mu_i \langle v_i, f\rangle u_i = \sum_{i=1}^{\infty} \langle u_i, g\rangle u_i, \tag{2-13}$$

and, since these functions are orthonormal, the solution of the equation takes the form

$$f(t) = \sum_{i=1}^{\infty} \frac{\langle u_i, g\rangle}{\mu_i} v_i. \tag{2-14}$$

Remark. *It is needed that the function g, as is established above, satisfy the following relation*

$$\sum_{i=1}^{\infty} \left(\frac{\langle u_i, g\rangle}{\mu_i}\right)^2 < \infty. \tag{2-15}$$

This relation is known as ***The Picard Condition****, and is important to ensure the solution f to be square integrable. In other words, the coefficients $\langle u_i, g\rangle$ must decay faster to zero than the singular values μ_i.*

Returning to **2-1**, the problems we are dealing with can be written in the way $Kf = g$, where seeking f will be the target, since K and g are given. The experimental data is often to have some level of noise and that leads to issues to approximate a solution of the problem. For dealing with that inconveniences it is possible to consider the finding of the function f, as an optimization process, in which the functional taken is

$$\rho(f) = \|Kf - g\|_2 . \tag{2-16}$$

The ill-conditioning of some well-established problems creates the necessity of finding a way to figure out a solution of them. There are some approximations to solve the inconveniences, and we point them out as in [21]

- Minimize $\rho(f)$ restricting the search of the solution to a subset S_f.
- Minimize $\rho(f)$ subject to the constraint that $\omega(f) < \delta$, being $\omega(\cdot)$ a measure of the *size* of f.
- Minimize $\omega(f)$, restricted to $\rho(f) < \alpha$.
- Minimize a linear combination of $\rho(f)^2$ and $\omega(f)^2$, i.e.:

  $$\min\left\{\rho(f)^2 + \lambda^2\omega(f)^2\right\}, \tag{2-17}$$

  where λ is a *penalty* factor.

The values, α, δ and λ are known as the regularization parameters, and function ω is often called the "smoothing norm".

2.2. Discrete Mollification

As a regularization tool, the mollification was developed in the decade of the 1980's and is exposed thoroughly in the texts [34] and [6]. It consists on convolution with a truncated gaussian kernels.

Given $\delta > 0$, $p > 0$ in $\mathbb{R}$, we define

$$A_{\delta p} = \left(\int_{B_{p/\delta}} exp(-x^2)dx\right)^{-1} \tag{2-18}$$

where

$$B_r := \{x \in \mathbb{R}/|x| < r\} \tag{2-19}$$

Now, we take a truncated Gaussian kernel:

$$\kappa_{\delta p}(x,y) = \begin{cases} A_{\delta p}\delta^{-2}exp(-x^2/\delta^2), & |x| \le p \\ 0, & |x| > p \end{cases} \tag{2-20}$$

Theorem 2.2.1. *This kernel satisfies*

- $\kappa \geq 0$.
- $\kappa \in C^\infty(B_p)$.
- $\kappa \equiv 0$ *outside* $\bar{B}_p$.
- $\int_{\mathbb{R}^n} \kappa_{\delta p} = 1$

Let $y = \{y_j\}_{j\in\mathbb{Z}}$ a discrete function which may consist of evaluations or cell averages of a real function $y = y(x)$ at equidistant grid points $x_j = x_0 + j\Delta x$, $\Delta x > 0$, $j \in \mathbb{Z}$.
The discrete mollification operator, applied to the discrete function y, is defined by the discrete convolution

$$[J_\eta y]_j = \sum_{i=-\eta}^{\eta} w_i y_{j-i}, \quad j \in \mathbb{Z}.$$

The support parameter $\eta \in \mathbb{Z}^+$ indicates the width of the mollification stencil, and the weights w_i satisfy $w_i = w_{-i}$ and $0 \leq w_i \leq w_{i-1}$ for $i = 1, \dots, \eta$ along with $\sum_{i=-\eta}^{\eta} w_i = 1$.
Discrete mollification is a convolution operator and as such, it requires η values to the right and to the left of any given point. For points close to the boundary, some extensions to exterior points of the domain are required. Several interesting options are presented in [4].
The weights w_i are defined in a precise way by integration of a certain truncated gaussian kernel ([6, 31]). Some weights are shown in Table **2-1**.

η	w_0	w_1	w_2	w_3	w_4	w_5
1	8.4272e-1	7.8640e-2				
2	6.0387e-1	1.9262e-1	5.4438e-3			
3	4.5556e-1	2.3772e-1	3.3291e-2	1.2099e-3		
4	3.6266e-1	2.4003e-1	6.9440e-2	8.7275e-3	4.7268e-4	
5	3.0028e-1	2.2625e-1	9.6723e-2	2.3430e-2	3.2095e-3	2.4798e-4

Table 2-1.: Mollification weights

The discrete mollification operator satisfies the following useful estimates.

Theorem 2.2.2. *(Theorem 2.2 of [1]) Let* $g \in C^4(\mathbb{R})$ *with* $g^{(4)}$ *bounded on* $\mathbb{R}$*, and set* $y_j = g(x_j)$*, where* $\{x_j\}_{j\in\mathbb{Z}}$ *is a uniform grid with discretization parameter* Δx*. If the data* $\{y_j^\varepsilon\}_{j\in\mathbb{Z}}$ *satisfy*

$$\left|y_j^\varepsilon - y_j\right| \leq \varepsilon \quad \textit{for all } j \in \mathbb{Z},$$

then

$$\left|[J_\eta y^\varepsilon]_j - [J_\eta y]_j\right| \le \varepsilon \quad \text{for all } j \in \mathbb{Z}.$$

Additionally, for each compact set $K = [a, b]$ there exists a constant $C = C(K)$ such that

$$\left|[J_\eta y]_j - g(x_j) - \frac{\Delta x^2}{2C_\eta} g''(x_j)\right| \le C\Delta x^4 \quad \text{for all } j \in \mathbb{Z}. \tag{2-21}$$

where $C_\eta := [2(\eta^2 w_\eta + (\eta-1)^2 w_{\eta-1} + \cdots + w_1) + w_0]^{-1}$.

Moreover, the following inequalities hold for all $j \in \mathbb{Z}$, where C is a different constant in each inequality:

$$\begin{aligned} \left|[J_\eta y]_j - g(x_j)\right| &\le C(\Delta x)^2, & \left|D_0 [J_\eta y]_j - (\Delta x) g'(x_j)\right| &\le C(\Delta x)^3, \\ \left|D_+ [J_\eta y]_j - (\Delta x) g'(x_j)\right| &\le C(\Delta x)^2, & \left|D_- D_+ [J_\eta y]_j - (\Delta x)^2 g''(x_j)\right| &\le C(\Delta x)^4. \end{aligned}$$

Where D_0, D_+ and D_- are the centered, forward and backward finite differences operators respectively.

The construction of a 2D kernel is analogous and details follow. However, we acknowledge the definition of 2D mollification by Acosta and Burger 2012 [5]. In this thesis we provide a new insight and more details.

Given $\delta > 0$, $p > 0$ in $\mathbb{R}$, we define

$$C_{\delta p} = \left(\int_{R_{p/\delta}} exp(-\|s\|^2) dx \right)^{-1} \tag{2-22}$$

where

$$R_r := \{ s \in \mathbb{R}^2 / \|s\|_\infty < r \} \tag{2-23}$$

Now, we take a truncated Gaussian kernel:

$$\phi_{\delta p}(s_1, s_2) = \begin{cases} C_{\delta p} \delta^{-2} exp(-(s_1^2 + s_2^2)/\delta^2), & \|(s_1, s_2)\|_\infty \le p \\ 0, & \|(s_1, s_2)\|_\infty > p \end{cases} \tag{2-24}$$

Theorem 2.2.3. *This kernel satisfies*

- $\phi \ge 0$.
- $\phi \in C^\infty(R_p)$.
- $\phi \equiv 0$ *outside* $\bar{R}_p$.
- $\int_{\mathbb{R}^2} \phi_{\delta p} = 1$

Definition 2.2.4. *Set $f : \mathbb{R}^2 \mapsto \mathbb{R}$ locally integrable, we define its δp-mollification in any t, denoted $J_{\delta p} f(t)$, as the convolution of f with $\phi_{\delta p}$ in t. That is,*

$$\begin{aligned} J_{\delta p} f(t) &= (\phi_{\delta p} * f)(t) && \text{(2-25)}\\ &= \int_{\mathbb{R}^2} \phi_{\delta p}(t-s) f(s) ds && \text{(2-26)}\\ &= \int_{R_p(t)} \phi_{\delta p}(t-s) f(s) ds && \text{(2-27)}\\ &= \int_{R_p} \phi_{\delta p}(-s) f(t+s) ds. && \text{(2-28)} \end{aligned}$$

Let $\Omega \subset \mathbb{R}^2$ a rectangle, $X = \{X_{ij}/X_{ij} = h(i,j), (i,j) \in \mathbb{Z}^2\} \cap \Omega$, a rectangular grid in Ω with step size $h \in \mathbb{R}^+$, and $G : X \mapsto \mathbb{R}$. Now we define some sets that will be of importance

$$\begin{aligned} S_{ij}(1) &= \frac{1}{2}\left(\begin{bmatrix} x_{i-1} \\ y_j \end{bmatrix} + \begin{bmatrix} x_i \\ y_j \end{bmatrix}\right) && \text{(2-29)}\\ S_{ij}(2) &= \frac{1}{2}\left(\begin{bmatrix} x_i \\ y_{j-1} \end{bmatrix} + \begin{bmatrix} x_i \\ y_j \end{bmatrix}\right) && \text{(2-30)}\\ I_{ij} &= [S_{ij}(1), S_{i+1,j}(1)) \times [S_{ij}(2), S_{i,j+1}(2)) && \text{(2-31)} \end{aligned}$$

We extend the function G to whole Ω, defining the function $\tilde{G}$ as follow

$$\tilde{G}(t) = \sum_{(i,j)\in\mathbb{Z}^2} \chi_{ij}(t) G(X_{ij}) \tag{2-32}$$

with χ_{ij} the characteristic function of the rectangle I_{ij}. Then for $\delta > 0$ and η a non negative integer, we define the $\delta\eta$-mollification of G as the δp- mollification of $\tilde{G}$ with

$$p = (\eta + 1/2)h \tag{2-33}$$

that is,

$$J_{\delta\eta} G(t) = J_{\delta p} \tilde{G}(t). \tag{2-34}$$

Henceforth, $p = 3\delta$. Notice that the function $\tilde{G}$ is constant over each of the rectangles I_{ij}, then the last definition can be written as follow

$$\begin{aligned} J_{\delta\eta} G(t) &= J_{\delta p} \tilde{G}(t) && \text{(2-35)}\\ &= \int_{R_p} \phi_{\delta p}(-s) \tilde{G}(t+s) ds && \text{(2-36)}\\ &= \int_{R_p} \phi_{\delta p}(-s) \sum_{(i,j)\in\mathbb{Z}^2} \chi_{ij}(t+s) G(X_{ij}) ds && \text{(2-37)}\\ &= \sum_{(i,j)\in\mathbb{Z}^2} G(X_{ij}) \int_{R_p} \phi_{\delta p}(-s) \chi_{ij}(t+s) ds && \text{(2-38)} \end{aligned}$$

We are interested on the mollification in the points of X, given a point X_{ij}, the mollification of G in it will be

$$J_{\delta\eta}G(X_{ij}) = J_{\delta p}\tilde{G}(X_{ij}) \tag{2-39}$$
$$= \int_{R_p} \phi_{\delta p}(-s)\tilde{G}(X_{ij}+s)ds \tag{2-40}$$
$$= \int_{R_p} \phi_{\delta p}(-s) \sum_{(m,n)\in\mathbb{Z}^2} \chi_{mn}(X_{ij}+s)G(X_{mn})ds \tag{2-41}$$
$$= \sum_{(m,n)\in\mathbb{Z}^2} G(X_{mn}) \int_{R_p} \phi_{\delta p}(-s)\chi_{mn}(X_{ij}+s)ds \tag{2-42}$$

The term $\phi_{\delta p}(-s)\chi_{ij}(X_{ij}+s)$ will be different from zero only when $\|s\|_\infty \leq p$ and $X_{ij}+s \in I_{mn}$, then basically we are taking the integral around the position X_{ij} over all intersections of the square of *radius* p and the rectangles I_{mn}, i.e. $\max\{|i-m|,|j-n|\} \leq \eta$. The figure 2.2 illustrates this issue:

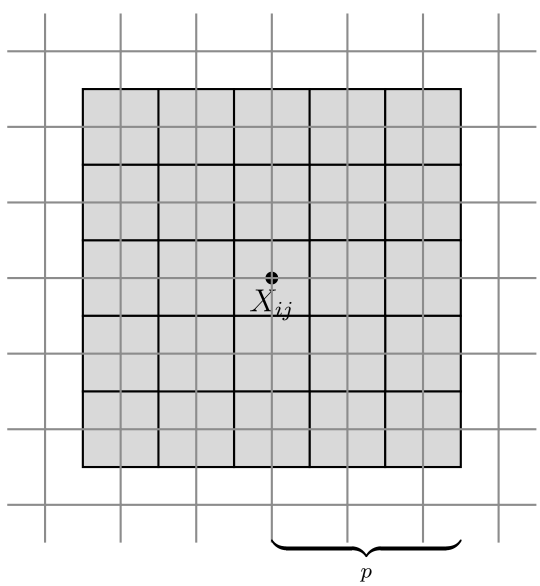

Figure 2-2.: The gray zones indicate where the integral is not zero.

Let $k = m - i$ and $l = n - j$, then

$$
\begin{aligned}
J_{\delta\eta}G(X_{ij}) &= \sum_{(m,n)\in\mathbb{Z}^2} G(X_{mn}) \int_{R_p} \phi_{\delta p}(-s)\chi_{mn}(X_{ij}+s)ds && \text{(2-43)}\\
&= \sum_{\substack{(k,l)\in\mathbb{Z}^2\\ \max\{|k|,|l|\}\le\eta}} G(X_{i+k,j+l}) \int_{R_p} \phi_{\delta p}(-s)\chi_{ij}(t+s)ds && \text{(2-44)}\\
&= \sum_{\substack{(k,l)\in\mathbb{Z}^2\\ \max\{|k|,|l|\}\le\eta}} w_{kl} G(X_{i+k,l+j}) && \text{(2-45)}
\end{aligned}
$$

where

$$
\begin{aligned}
w_{kl} &= \int_{I_{kl}} \phi_{\delta p}(-s)ds && \text{(2-46)}\\
&= \int_{X_k-h/2}^{X_l+h/2}\int_{y_l-h/2}^{y_l+h/2} \phi_{\delta p}(x,y)dxdy && \text{(2-47)}\\
&= \int_{X_k-h/2}^{X_l+h/2}\int_{y_l-h/2}^{y_l+h/2} C_{\delta p}\delta^{-2}exp(-(x^2+y^2)/\delta^2)dxdy && \text{(2-48)}\\
&= C_{\delta p}\delta^{-2}\int_{x_k-h/2}^{x_l+h/2}\int_{y_l-h/2}^{y_l+h/2} exp(-x^2/\delta^2)exp(-y^2/\delta^2)dxdy && \text{(2-49)}\\
&= C_{\delta p}\delta^{-2}\int_{x_k-h/2}^{x_k+h/2} exp(-x^2/\delta^2)dx \int_{y_l-h/2}^{y_l+h/2} exp(-y^2/\delta^2)dy && \text{(2-50)}\\
&= \omega_l\omega_k && \text{(2-51)}
\end{aligned}
$$

and

$$
\begin{aligned}
\omega_k &= \frac{1}{2}\left(erf\left(\frac{x_k+\frac{h}{2}}{\delta}\right) - erf\left(\frac{x_k-\frac{h}{2}}{\delta}\right)\right) && \text{(2-52)}\\
\omega_l &= \frac{1}{2}\left(erf\left(\frac{y_l+\frac{h}{2}}{\delta}\right) - erf\left(\frac{y_l-\frac{h}{2}}{\delta}\right)\right) && \text{(2-53)}
\end{aligned}
$$

Lemma 2.2.5.

$$
\sum_{\max\{|k|,|l|\}\le\eta} k w_{kl} = 0 \quad and \quad \sum_{\max\{|k|,|l|\}\le\eta} l w_{kl} = 0. \tag{2-54}
$$

Proof.

$$
\begin{aligned}
\sum_{\max\{|k|,|l|\}\le\eta} k w_{kl} &= \sum_{\max\{|k|,|l|\}\le\eta} k w_{kl} && \text{(2-55)}\\
&= \sum_{\max\{|k|,|l|\}\le\eta} k w_k w_l && \text{(2-56)}\\
&= \sum_{l=-\eta}^{\eta}\left(\sum_{k=-\eta}^{\eta} k w_k\right) w_l = 0. && \text{(2-57)}
\end{aligned}
$$

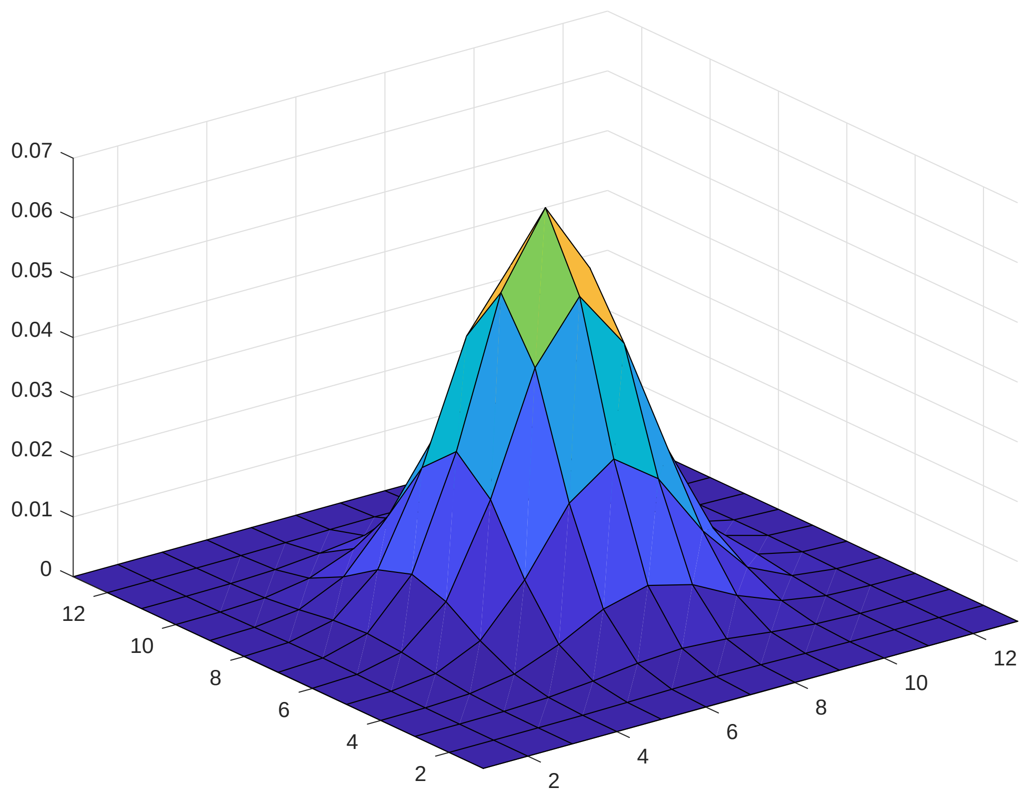

Figure 2-3.: The w's for $h = 0.01, \delta = 0.2$ and $\eta = 4$

□

Definition 2.2.6. *A function g is called Lipschitz continuous, if there exists a constant C_{Lip} such that*

$$\|g(x_1) - g(x_2)\| \leq C_{Lip}\|x_1 - x_2\| \tag{2-58}$$

Remark. *From now on, the function g will be assumed Lipschitz continuous.*

Theorem 2.2.7. *If $g_x \in C^{0,1}(\mathbb{R}^2)$ in the x variable. Then there exists a constant C, independent of δ, such that*

$$\|(J_{\delta\eta}G)_x - g_x\|_\infty \ \leq \ C\left(\delta + \frac{h}{\delta}\right), \tag{2-59}$$

where h and δ are independent.

Proof. By the triangle inequality,

$$\|(J_{\delta\eta}G)_x - g_x\|_\infty \ \leq \ \|(J_{\delta\eta}g)_x - (J_{\delta\eta}G)_x\|_\infty + \|(J_{\delta\eta}g)_x - g_x\|_\infty \tag{2-60}$$

We estimate each term separately. Then, for the first one

$$|(J_{\delta\eta}g(x,y))_x - (J_{\delta\eta}G(x,y))_x| = \left|\frac{\partial}{\partial x}\left(J_{\delta\eta}g(x,y) - J_{\delta\eta}G(x,y)\right)\right| \tag{2-61}$$

$$= \left|\frac{\partial}{\partial x}\left(\int_{R_p(x,y)} \phi_{\delta p}(x-s_1, y-s_2)(g(s) - G(s))ds\right)\right|$$

$$= \left|\frac{\partial}{\partial x}\left(\int_{R_p(x,y)} \phi_{\delta p}(x-s_1, y-s_2)(g(s) - G(s))ds\right)\right|$$

$$= \left|\frac{\partial}{\partial x}\left(\int_{y-p}^{y+p}\int_{x-p}^{x+p} \phi_{\delta p}(x-s_1, y-s_2)(g(s) - G(s))ds\right)\right|$$

$$= \left|\int_{y-p}^{y+p}\frac{\partial}{\partial x}\left(\int_{x-p}^{x+p} \phi_{\delta p}(x-s_1, y-s_2)(g(s) - G(s))ds\right)\right|$$

$$= \left|\int_{y-p}^{y+p}\int_{x-p}^{x+p}\frac{\partial}{\partial x}\left(\phi_{\delta p}(x-s_1, y-s_2)\right)(g(s) - G(s))ds\right.$$

$$+ \int_{y-p}^{y+p}\phi_{\delta p}(-p, y-s_2)(g(x+p, s_2) - G(x+p, s_2))ds_2$$

$$\left.- \int_{y-p}^{y+p}\phi_{\delta p}(p, y-s_2)(g(x-p, s_2) - G(x-p, s_2))ds_2\right|$$

$$\leq \int_{y-p}^{y+p}\int_{x-p}^{x+p}\left|\frac{\partial}{\partial x}\left(\phi_{\delta p}(x-s_1, y-s_2)\right)(g(s) - G(s))\right| ds \tag{2-62}$$

$$+ \int_{y-p}^{y+p}\left|\phi_{\delta p}(-p, y-s_2)(g(x+p, s_2) - G(x+p, s_2))\right| ds_2 \tag{2-63}$$

$$+ \int_{y-p}^{y+p}\left|\phi_{\delta p}(p, y-s_2)(g(x-p, s_2) - G(x-p, s_2))\right| ds_2 \tag{2-64}$$

Taking (2-62) term we have

$$\int_{y-p}^{y+p}\int_{x-p}^{x+p}\left|\frac{\partial}{\partial x}\left(\phi_{\delta p}(x-s_1,y-s_2)\right)\left(g(s)-G(s)\right)\right|ds \leq$$
$$\leq C_{Lip}h\int_{y-p}^{y+p}\int_{x-p}^{x+p}\frac{C_{\delta p}}{\delta^2}\left|\frac{-2(x-s_1)}{\delta^2}exp\left(\frac{-(x-s_1)^2-(y-s_2)^2}{\delta^2}\right)\right|ds_1ds_2$$
$$=\frac{2C_{Lip}hC_{\delta p}}{\delta^2}\int_{y-p}^{y+p}exp\left(\frac{-(y-s_2)^2}{\delta^2}\right)ds_2\int_{x-p}^{x+p}\left|\frac{-2(x-s_1)}{\delta^2}exp\left(\frac{-(x-s_1)^2}{\delta^2}\right)\right|ds_1$$
$$=\frac{2C_{Lip}hC_{\delta p}}{\delta^2}\int_{y-p}^{y+p}exp\left(\frac{-(y-s_2)^2}{\delta^2}\right)ds_2\left(2\int_{x}^{x+p}\frac{-2(x-s_1)}{\delta^2}exp\left(\frac{-(x-s_1)^2}{\delta^2}\right)ds_1\right)$$
$$=\frac{2C_{Lip}hC_{\delta p}}{\delta^2}\int_{y-p}^{y+p}exp\left(\frac{-(y-s_2)^2}{\delta^2}\right)ds_2\left(2\int_{0}^{p^2/\delta^2}exp(-t)dt\right)$$
$$=\frac{4C_{Lip}hC_{\delta p}}{\delta^2}\left(1-exp(-p^2/\delta^2)\right)\int_{y-p}^{y+p}exp\left(\frac{-(y-s_2)^2}{\delta^2}\right)ds_2$$
$$=\frac{4C_{Lip}hC_{\delta p}}{\delta^2}\left(1-exp(-p^2/\delta^2)\right)\delta\int_{-p/\delta}^{p/\delta}exp\left(t^2\right)dt$$
$$=\frac{4C_{Lip}h}{\delta}\frac{\left(1-exp(-p^2/\delta^2)\right)}{\int_{-p/\delta}^{p/\delta}exp(-x^2)dx}\cdot\frac{\int_{-p/\delta}^{p/\delta}exp(-t^2)dt}{\int_{-p/\delta}^{p/\delta}exp(-y^2)dy}$$
$$\leq\frac{4C_{Lip}A_{\delta p}h}{\delta}.$$

where $A_{\delta p}=1/\int_{-p/\delta}^{p/\delta}exp(-x^2)dx$ as it was defined in the one dimensional sense.
For (2-63) + (2-64) we have

$$\int_{y-p}^{y+p}\left|\phi_{\delta p}(-p,y-s_2)(g(x+p,s_2)-G(x+p,s_2))\right|ds_2+$$
$$+\int_{y-p}^{y+p}\left|\phi_{\delta p}(p,y-s_2)(g(x-p,s_2)-G(x-p,s_2))\right|ds_2\leq$$
$$\leq 4C_{Lip}h\int_{y-p}^{y+p}\frac{C_{\delta p}}{\delta^2}exp\left(\frac{-p^2-(y-s_2)^2}{\delta^2}\right)ds_2$$
$$=\frac{4C_{Lip}hC_{\delta p}}{\delta^2}exp(-p^2/\delta^2)\int_{y-p}^{y+p}exp\left(\frac{-(y-s_2)^2}{\delta^2}\right)ds_2$$
$$=\frac{4C_{Lip}hA_{\delta p}}{\delta^2}exp(-p^2/\delta^2)\cdot\frac{\delta\int_{-p/\delta}^{p/\delta}exp(-t^2)dt}{\int_{-p/\delta}^{p/\delta}exp(-y^2)dy}$$
$$\leq\frac{4C_{Lip}A_{\delta p}h}{\delta}.$$

Then, we have that

$$\|(J_{\delta\eta}g)_x-(J_{\delta\eta}G)_x\|_\infty\leq\frac{8C_{Lip}A_{\delta p}h}{\delta}. \tag{2-65}$$

Now, if $f = g_x$, then

$$\begin{aligned}
|J_{\delta p}f(x,y) - f(x,y)| &= \left| \int_{R_p} \phi(-s)\left(f(x+s_1, y+s_2) - f(x,y)\right) ds \right| \\
&\leq \int_{-p}^{p}\int_{-p}^{p} \frac{C_{\delta p}}{\delta^2} exp\left(\frac{-s_1^2 - s_2^2}{\delta^2}\right) |f(x+s_1, y+s_2) - f(x,y)| \\
&\leq \frac{C_{Lip}C_{\delta p}}{\delta^2} \int_{-p}^{p}\int_{-p}^{p} (|s_1| + |s_2|) exp\left(\frac{-s_1^2 - s_2^2}{\delta^2}\right) ds_1 ds_2 \\
&= \frac{C_{Lip}C_{\delta p}}{\delta^2} \int_{-p}^{p}\int_{-p}^{p} |s_1| exp\left(\frac{-s_1^2 - s_2^2}{\delta^2}\right) + |s_2| exp\left(\frac{-s_1^2 - s_2^2}{\delta^2}\right) ds_1 ds_2 \\
&= \frac{C_{Lip}C_{\delta p}}{\delta^2} \left[\int_{-p}^{p} |s_1| exp\left(\frac{-s_1^2}{\delta^2}\right) ds_1 \int_{-p}^{p} exp\left(\frac{-s_2^2}{\delta^2}\right) ds_2 \right. \\
&\quad \left. + \int_{-p}^{p} |s_2| exp\left(\frac{-s_2^2}{\delta^2}\right) ds_2 \int_{-p}^{p} exp\left(\frac{-s_1^2}{\delta^2}\right) ds_1 \right] \\
&\leq \frac{C_{Lip}C_{\delta p}}{\delta^2} \left(\frac{\delta}{A_{\delta p}}\delta^2 + \frac{\delta}{A_{\delta p}}\delta^2 \right) = 2C_{Lip}A_{\delta p}\delta
\end{aligned}$$

We conclude

$$\|(J_{\delta p}G)_x - g_x\|_\infty \leq C\left(\delta + \frac{h}{\delta}\right) \tag{2-66}$$

□

Theorem 2.2.8. *Given G and G^ϵ are defined on K, and satisfy $\|G - G^\epsilon\|_\infty \leq \epsilon$, then*

$$\|(J_{\delta p}G)_x - (J_{\delta p}G^\epsilon)_x\|_\infty \leq C\frac{\epsilon}{\delta}$$

Proof.

$$\begin{aligned}
|(J_{\delta p}G)_x - (J_{\delta p}G^\epsilon)_x| &= \left| \frac{\partial}{\partial x} \int_{R_p(x,y)} \phi_{\delta p}(x - s_1, y - s_2)(G(s_1, s_2) - G^\epsilon(s_1, s_2)) ds_1 d_2 \right| \\
&= \left| \int_{y-p}^{y+p} \frac{\partial}{\partial x} \int_{x-p}^{x+p} \phi_{\delta p}(x - s_1, y - s_2)(G(s_1, s_2) - G^\epsilon(s_1, s_2)) ds_1 d_2 \right| \\
&= \left| \int_{y-p}^{y+p} \phi_{\delta p}(-p, y - s_2)(G(x+p, s_2) - G^\epsilon(x+p, s_2)) ds_2 \right. \\
&\quad - \int_{y-p}^{y+p} \phi_{\delta p}(p, y - s_2)(G(x-p, s_2) - G^\epsilon(x-p, s_2)) ds_2 \\
&\quad \left. + \int_{y-p}^{y+p}\int_{x-p}^{x+p} \frac{\partial}{\partial x}\left(\phi_{\delta p}(x - s_1, y - s_2)\right)(G(s_1, s_2) - G^\epsilon(s_1, s_2)) ds_1 d_2 \right|
\end{aligned}$$

$$\begin{aligned}
&\leq \epsilon \int_{y-p}^{y+p} \phi_{\delta p}(-p, y-s_2) ds_2 + \epsilon \int_{y-p}^{y+p} \phi_{\delta p}(p, y-s_2) ds_2 \\
&\quad + \frac{\epsilon C_{\delta p}}{\delta^2} \int_{y-p}^{y+p} \int_{x-p}^{x+p} \left| \frac{-2(x-s_1)}{\delta^2} exp\left(\frac{-(x-s_1)^2 - (y-s_2)^2}{\delta^2} \right) \right| ds_1 ds_2 \\
&\leq \frac{2\epsilon A_{\delta p}}{\delta^2} \delta + \frac{2\epsilon A_{\delta p}}{\delta^2} \delta = \frac{4\epsilon A_{\delta p}}{\delta^2} \delta
\end{aligned}$$

□

We conclude

$$\begin{aligned}
\|(J_{\delta p} G^\epsilon)_x - (J_{\delta p} g)_x\|_\infty &\leq \|(J_{\delta p} G^\epsilon)_x - (J_{\delta p} G)_x\|_\infty + \|(J_{\delta p} G)_x - (J_{\delta p} g)_x\|_\infty \quad (2\text{-}67) \\
&\leq \frac{C}{\delta}(\epsilon + h) \quad (2\text{-}68)
\end{aligned}$$

moreover

$$\|(J_{\delta p} G^\epsilon)_x - g_x\|_\infty \leq C\left(\delta + \frac{\epsilon}{\delta} + \frac{h}{\delta} \right) \quad (2\text{-}69)$$

From the last theorems, we obtain

$$\|D_0(J_{\delta p} G^\epsilon) - g_x\|_\infty \leq \|(J_{\delta p} G^\epsilon)_x - g_x\|_\infty + \|D_0(J_{\delta p} G^\epsilon) - (J_{\delta p} G^\epsilon)_x\|_\infty \quad (2\text{-}70)$$

It is necessary that there exist a bound for the central difference, the next result establish it.

Theorem 2.2.9. *If G is a bounded function, then*

$$\|D_0(J_{\delta p} G)\|_\infty \leq 2\frac{A_{\delta p}}{\delta} \|G\|_\infty \quad (2\text{-}71)$$

Proof.

$$\begin{aligned}
|D_0(J_{\delta p} G)(x,y)| &= \frac{1}{2h} |J_{\delta p} G(x+h, y) - J_{\delta p} G(x-h, y)| \\
&= \frac{1}{2h} \left| \int_{\mathbb{R}^2} \left(\phi_{\delta p}(x+h-s_1, y) - \phi_{\delta p}(x-h-s_1, y) \right) G(s_1, s_2) ds_1 ds_2 \right| \\
&\leq \frac{1}{2h} \frac{\|G\|_\infty C_{\delta p}}{\delta^2} \left(\int_{y-p}^{y+p} exp\left(\frac{-(y-s_2)^2}{\delta^2} \right) ds_2 \right) \cdot \\
&\quad \cdot \left(\int_{x-h-p}^{x+h+p} \left| exp\left(\frac{-(x+h-s_1)^2}{\delta^2} \right) - exp\left(\frac{-(x-h-s_1)^2}{\delta^2} \right) \right| ds_1 \right) \\
&= \frac{\|G\|_\infty A_{\delta p}}{2h\delta} \int_{-h-p}^{h+p} \left| exp\left(\frac{-(-z+h)^2}{\delta^2} \right) - exp\left(\frac{-(-z-h)^2}{\delta^2} \right) \right| dz \\
&= \frac{\|G\|_\infty A_{\delta p}}{2h\delta} \int_{-h-p}^{h+p} \left| exp\left(\frac{-(z+h)^2}{\delta^2} \right) - exp\left(\frac{-(z-h)^2}{\delta^2} \right) \right| dz \\
&= \frac{\|G\|_\infty A_{\delta p}}{2h\delta} 2 \int_{-h-p}^{0} exp\left(\frac{-(z+h)^2}{\delta^2} \right) - exp\left(\frac{-(z-h)^2}{\delta^2} \right) dz
\end{aligned}$$

Now, using a generalized mean value theorem: if $f \in C[a-h, b+h]$, then there exist constants θ_i, with $|\theta_i| \leq 1$, $i = 1, 2$, such that

$$\int_a^b (f(x+h) - f(x-h))dx = 2h(f(b+\theta_1 h) - f(a-\theta_2 h)) \tag{2-72}$$

finally, we get

$$\begin{aligned} |D_0(J_{\delta p}G)(x,y)| &\leq \frac{2A_{\delta p}\|G\|_\infty}{\delta}\left(exp\left(\frac{-(\theta_1 h)^2}{\delta^2}\right) - exp\left(\frac{-(-h-p-\theta_2 h)^2}{\delta^2}\right)\right) \\ &\leq \frac{2A_{\delta p}\|G\|_\infty}{\delta} \end{aligned}$$

□

Theorem 2.2.10. *If the function $g_{xx} \in C^{0,1}\Omega$, then*

$$\|(J_{\delta p}G^\epsilon)_{xx} - g_{xx}\|_\infty \leq C_1\delta + \frac{24C_2 h}{\delta^2} + \frac{24C_3\epsilon}{\delta^2} \tag{2-73}$$

Proof.

$$\begin{aligned} \|(J_{\delta p}G^\epsilon)_{xx} - g_{xx}\|_\infty &\leq \|(J_{\delta p}G^\epsilon)_{xx} - (J_{\delta p}G)_{xx}\|_\infty + \|(J_{\delta p}G)_{xx} - (J_{\delta p}g)_{xx}\|_\infty \\ &\quad + \|(J_{\delta p}g)_{xx} - g_{xx}\|_\infty \end{aligned}$$

For the last term, trivially

$$\|(J_{\delta p}g)_{xx} - g_{xx}\|_\infty = \|(J_{\delta p}g_{xx}) - g_{xx}\|_\infty \leq C_1\delta \tag{2-74}$$

Then we take the middle one

$$\begin{aligned} \left|\frac{\partial^2}{\partial x^2}(J_{\delta p}G(x,y)) - \frac{\partial^2}{\partial x^2}(J_{\delta p}g(x,y))\right| &= \left|\frac{\partial}{\partial x}\left(\frac{\partial}{\partial x}(J_{\delta p}(G-g)(x,y))\right)\right| = \\ = \left|\frac{\partial}{\partial x}\left(\int_{y-p}^{y+p} \phi_{\delta p}(-p, y-s_2)(G(x+p,s_2) - g(x+p,s_2))ds_2\right.\right. \\ - \int_{y-p}^{y+p} \phi_{\delta p}(p, y-s_2)(G(x-p,s_2) - g(x-p,s_2))ds_2 \\ \left.\left. + \int_{y-p}^{y+p}\int_{x-p}^{x+p}\left(\frac{\partial}{\partial x}\phi_{\delta p}(x-s_1, y-s_2)\right)(G(s_1,s_2) - g(s_1,s,2))s_1 ds_2\right)\right| \end{aligned}$$

The first two integrals vanished under the derivative and from the last one we get

$$\begin{aligned} \left|\frac{\partial^2}{\partial x^2}(J_{\delta p}G(x,y)) - \frac{\partial^2}{\partial x^2}(J_{\delta p}g(x,y))\right| = \\ \left|\int_{y-p}^{y+p}\left(\frac{\partial}{\partial x}\phi_{\delta p}(-p, y-s_2)\right)(G(x+p,s_2) - g(x+p,s_2))ds_2\right. \\ - \int_{y-p}^{y+p}\left(\frac{\partial}{\partial x}\phi_{\delta p}(p, y-s_2)\right)(G(x-p,s_2) - g(x-p,s_2))ds_2 \\ \left. + \int_{y-p}^{y+p}\int_{x-p}^{x+p}\left(\frac{\partial^2}{\partial x^2}\phi_{\delta p}(x-s_1, y-s_2)\right)(G(s_1,s_2) - g(s_1,s_2))ds_1 ds_2\right| \end{aligned}$$

Again, we analyze these integrals separately

$$\left|\int_{y-p}^{y+p}\left(\frac{\partial}{\partial x}\phi_{\delta p}(-p,y-s_2)\right)(G(x+p,s_2)-g(x+p,s_2))ds_2\right| \leq \tag{2-75}$$

$$\leq \frac{C_{\delta p}}{\delta^2}\left|\int_{y-p}^{y+p}\left(\frac{2p}{\delta^2}exp\left(\frac{-p^2-(y-s_2)^2}{\delta^2}\right)\right)(G(x+p,s_2)-g(x+p,s_2))ds_2\right| \tag{2-76}$$

$$\leq \frac{2pC_{\delta p}C_{Lip}h}{\delta^4}exp\left(\frac{-p^2}{\delta^2}\right)\int_{y-p}^{y+p}exp\left(\frac{-(y-s_2)^2}{\delta^2}\right)ds_2 \tag{2-77}$$

$$\leq \frac{2pC_{\delta p}C_{Lip}h}{\delta^4}\frac{\delta}{A_{\delta p}}exp\left(\frac{-p^2}{\delta^2}\right) \leq \frac{2\cdot 3\delta C_{\delta p}C_{Lip}h}{\delta^4}\frac{\delta}{A_{\delta p}} \leq \frac{6A_{\delta p}C_{Lip}h}{\delta^2} \tag{2-78}$$

This inequality can be established as well for the term

$$\left|\int_{y-p}^{y+p}\left(\frac{\partial}{\partial x}\phi_{\delta p}(p,y-s_2)\right)(G(x-p,s_2)-g(x-p,s_2))ds_2\right| \leq \frac{6A_{\delta p}C_{Lip}h}{\delta^2} \tag{2-79}$$

The integral involving the second derivative

$$\left|\int_{y-p}^{y+p}\int_{x-p}^{x+p}\left(\frac{\partial^2}{\partial x^2}\phi_{\delta p}(x-s_1,y-s_2)\right)(G(s_1,s_2)-g(s_1,s_2))ds_1ds_2\right| \leq$$

$$\int_{y-p}^{y+p}\int_{x-p}^{x+p}\left(\frac{\partial^2}{\partial x^2}\phi_{\delta p}(x-s_1,y-s_2)\right)\left|G(s_1,s_2)-g(s_1,s_2)\right|ds_1ds_2 \leq$$

$$C_{Lip}h\int_{y-p}^{y+p}\int_{x-p}^{x+p}\left|\frac{\partial^2}{\partial x^2}\phi_{\delta p}(x-s_1,y-s_2)\right|ds_1ds_2 \leq$$

$$\frac{C_{\delta p}C_{Lip}h}{\delta^2}\left(\int_{y-p}^{y+p}exp\left(\frac{-(y-s_2)^2}{\delta^2}\right)ds_2\right)\cdot$$

$$\cdot\left(\int_{x-p}^{x+p}\left|exp\left(\frac{-(x-s_1)^2}{\delta^2}\right)\left(\frac{-2}{\delta^2}+\frac{4(x-s_1)^2}{\delta^4}\right)\right|ds_1\right) \leq$$

$$\frac{C_{\delta p}C_{Lip}h}{\delta^2}\frac{\delta}{A_{\delta p}}\left(\int_{-p}^{p}\left|exp\left(\frac{-t^2}{\delta^2}\right)\left(\frac{-2}{\delta^2}+\frac{4t^2}{\delta^4}\right)\right|dt\right) \leq$$

$$\frac{A_{\delta p}C_{Lip}h}{\delta}\left(\frac{4t}{\delta^2}exp\left(\frac{-t^2}{\delta^2}\right)\right)\Bigg|_0^p = \frac{4A_{\delta p}C_{Lip}h}{\delta}\frac{p}{\delta^2} = \frac{4A_{\delta p}C_{Lip}h}{\delta}\frac{3\delta}{\delta^2} = \frac{12A_{\delta p}C_{Lip}h}{\delta^2}$$

That implies

$$\|(J_{\delta p}G)_{xx}-(J_{\delta p}g)_{xx}\|_\infty \leq \frac{24C_2h}{\delta^2} \tag{2-80}$$

Now we need to estimate the first term. Following the same ideas bellow, we obtain

$$\left|\frac{\partial^2}{\partial x^2}(J_{\delta p}G^\epsilon)(x,y)-\frac{\partial^2}{\partial x^2}(J_{\delta p}G)(x,y)\right| \leq \frac{24C_3\epsilon}{\delta^2} \tag{2-81}$$

□

Theorem 2.2.11. *Let $g \in C^4(\mathbb{R}^2)$ and M a bound for g and its derivatives up to fourth order. Let G be the discrete version of g defined on $X = \{X_{ij}/X_{ij} = h(i,j), (i,j) \in \mathbb{Z}^2\} \cap \Omega$.*
Stability and Consistency. *If G^ϵ is defined on X such that*

$$|G^\epsilon(X_{ij}) - G(X_{ij})| \leq \epsilon, \qquad X_{ij} \in X, \tag{2-82}$$

then for each compact set $K = [a,b] \times [c,d]$ there exist a constant C_K such that if $X_{ij} \in K$

$$|J_{\delta\eta}G^\epsilon(X_{ij}) - J_{\delta\eta}G(X_{ij})| \leq \epsilon, \tag{2-83}$$

$$|J_{\delta\eta}G^\epsilon(X_{ij}) - g(X_{ij})| \leq C_K h^2. \tag{2-84}$$

Numerical Differentiation with mollification: *Moreover:*

$$\left| D_+ J_{\delta\eta} G(X_{ij}) - \frac{\partial}{\partial x}(X_{ij}) \right| \leq Ch, \tag{2-85}$$

$$\left| D_0 J_{\delta\eta} G(X_{ij}) - \frac{\partial}{\partial x} g(X_{ij}) \right| \leq Ch^2 \tag{2-86}$$

$$\left| D_- D_+ J\delta\eta G(X_{ij}) - \frac{\partial^2}{\partial x^2} g(X_{ij}) \right| \leq Ch^2, \tag{2-87}$$

where D_+, D_- and D_0 are the forward, backward and central operators of discrete differentiation in x respectively. The last inequalities are true for the second variable as well.

Proof. **Stability:**

$$|J_{\delta\eta}G^\epsilon(X_{ij}) - J_{\delta\eta}G(X_{ij})| = \left| \sum_{\max\{|k|,|l|\} \leq \eta} w_{kl} \left(G^\epsilon(X_{ij}) - G(X_{ij}) \right) \right| \tag{2-88}$$

$$\leq \sum_{\max\{|k|,|l|\} \leq \eta} w_{kl} \left| G^\epsilon(X_{ij}) - G(X_{ij}) \right| \tag{2-89}$$

$$= |G^\epsilon(X_{ij}) - G(X_{ij})| \sum_{\max\{|k|,|l|\} \leq \eta} w_{kl} \leq \epsilon \tag{2-90}$$

Consistency: let $X_{ij} \in K$ then for Taylor's Theorem, for each $(k,l) \in \mathbb{Z}^2$, with $\max\{|k|,|l|\} \leq \eta$, there exists $R_{kl} \in [a+p, b-p] \times [c+p, d-p]$ such that

$$g(X_{i+k,j+l}) = g(X_{ij}) + hk\frac{\partial}{\partial x} g(X_{ij}) + hl\frac{\partial}{\partial y} g(X_{ij}) + \frac{h^2}{2} R_{kl} \tag{2-91}$$

Thus

$$\begin{aligned} J_{\delta\eta}G(X_{ij}) &= \sum_{\max\{|k|,|l|\} \leq \eta} w_{kl} g(X_{i+k,j+l}) \\ &= \sum_{\max\{|k|,|l|\} \leq \eta} w_{kl} \left(g(X_{ij}) + h\left(k\frac{\partial}{\partial x} g(X_{ij}) + l\frac{\partial}{\partial y} g(X_{ij}) \right) + \frac{h^2}{2} R_{kl} \right) \\ &= g(X_{ij}) + \frac{h^2}{2} \sum_{\max\{|k|,|l|\} \leq \eta} w_{kl} R_{kl} \end{aligned}$$

from the last lemma Here the term R_{kl} represents the remainder in Taylor's Theorem for multivariate functions.

Numerical Differentiation: If $X_{i-1,j}, X_{i+1,j} \in K$, there exist $R_{k,l}$ and $Q_{k,l}$, being the remainders in Taylor's Theorem of fourth order, such that

$$\begin{aligned}
J_{\delta\eta}G(X_{i-1,j}) &= g(X_{i-1,j}) + \frac{h^4}{24}\sum_{l=-\eta}^{\eta}\sum_{k=-\eta}^{\eta} w_{k,l}R_{k,l} \\
&+\frac{h^2}{2}\sum_{l=-\eta}^{\eta}\sum_{k=-\eta}^{\eta} w_{k,l}\left(k^2\frac{\partial^2}{\partial x^2}g(X_{i-1,j}) + kl\frac{\partial^2}{\partial x\partial y}g(X_{i-1,j}) + l^2\frac{\partial^2}{\partial y^2}g(X_{i-1,j})\right) \\
J_{\delta\eta}G(X_{i+1,j}) &= g(X_{i+1,j}) + \frac{h^4}{24}\sum_{l=-\eta}^{\eta}\sum_{k=-\eta}^{\eta} w_{k,l}Q_{k,l} \\
&+\frac{h^2}{2}\sum_{l=-\eta}^{\eta}\sum_{k=-\eta}^{\eta} w_{k,l}\left(k^2\frac{\partial^2}{\partial x^2}g(X_{i+1,j}) + kl\frac{\partial^2}{\partial x\partial y}g(X_{i+1,j}) + l^2\frac{\partial^2}{\partial y^2}g(X_{i+1,j})\right)
\end{aligned}$$

The last equations are consequence of Taylor's Theorem for the variable x.
Now, for some υ_i and ν_i between $X_{i-1,j}$ and $X_{i+1,j}$ we have

$$\left|\frac{g(X_{i+1,j}) - g(X_{i-1,j})}{2h} - \frac{\partial}{\partial x}g(X_{i,j})\right| = \frac{h^2}{12}\left|\frac{\partial^3}{\partial x^3}g(\upsilon_i)\right| \leq \frac{h^2}{12}M \tag{2-92}$$

$$\left|\frac{\frac{\partial^2}{\partial x^2}g(X_{i+1,j}) - \frac{\partial^2}{\partial x^2}g(X_{i-1,j})}{2h}\right| = \left|\frac{\partial^3}{\partial x^3}g(\nu_i)\right| \leq M \tag{2-93}$$

$$\left|\frac{\frac{\partial^4}{\partial x^4}g(X_{i+1,j}) - \frac{\partial^4}{\partial x^4}g(X_{i-1,j})}{2h}\right| \leq \frac{M}{h} \tag{2-94}$$

For these and other similar estimates, we have

$$\frac{J_{\delta\eta}G(X_{i+1,j}) - J_{\delta\eta}G(X_{i-1,j})}{2h} = \frac{\partial}{\partial x}g(X_{i,j}) + O(h^2) \tag{2-95}$$

The other estimates can be obtained in similar way. □

Theorem 2.2.12. *With the hypothesis of the theorem above, the next inequalities are obtained*

$$\left|D_+J_{\delta\eta}G^\epsilon(X_{i,j}) - \frac{\partial}{\partial x}g(X_{i,j})\right| \leq 2\left(\frac{\epsilon}{h}\right) + Ch \tag{2-96}$$

$$\left|D_0J_{\delta\eta}G^\epsilon(X_{i,j}) - \frac{\partial}{\partial x}g(X_{i,j})\right| \leq \left(\frac{\epsilon}{h}\right) + Ch^2 \tag{2-97}$$

$$\left|D_-D_+J_{\delta\eta}G^\epsilon(X_{i,j}) - \frac{\partial^2}{\partial x^2}g(X_{i,j})\right| \leq 4\left(\frac{\epsilon}{h^2}\right) + Ch^2 \tag{2-98}$$

Proof. Only one of the proofs is shown here:

$$\begin{aligned}
\left|D_+J_{\delta\eta}G^{\epsilon}(X_{i,j}) - \frac{\partial}{\partial x}g(X_{i,j})\right| &\leq |D_+J_{\delta\eta}G^{\epsilon}(X_{i,j}) - D_+J_{\delta\eta}G(X_{i,j})| + \left|D_+J_{\delta\eta}G(X_{i,j})\frac{\partial}{\partial x}g(X_{i,j})\right| \\
&\leq \frac{1}{h}\left|J_{\delta\eta}G^{\epsilon}(X_{i+1,j}) - J_{\delta\eta}G(X_{i+1,j})\right| \\
&\quad + \frac{1}{h}\left|J_{\delta\eta}G^{\epsilon}(X_{i-1,j}) - J_{\delta\eta}G(X_{i-1,j})\right| \\
&\quad + \left|D_+J_{\delta\eta}G(X_{i,j})\frac{\partial}{\partial x}g(X_{i,j})\right| \\
&\leq 2\left(\frac{\epsilon}{h}\right) + Ch
\end{aligned}$$

□

Inverse problems and regularization play important roles in this thesis and so do fractional derivatives, introduced in the next chapter.

3. Fractional Derivatives

In the classical calculus the derivatives play a fundamental role and their applications can be found in many fields as physics, chemistry, economics, etc. The order of the derivatives represents a core topic in any model concerning differential equations and the questioning about the possibilities of that order for not being integer and its implications in the modelling, will be the aim of this chapter.
In 1695 Leibniz wrote a letter to L'Hôpital putting on the table a possible generalization of the concept of derivative introducing the non-integer order. Then L'Hôpital asked for the results if the order was $n = 1/2$, which Leibniz later responded "one day, useful consequences will be drawn" [29]. Those questions were addressed in works of mathematicians as Lacroix, Abel and Fourier, lately the fractional calculus acquired relevancy for its applications in engineering.
There are different definitions of fractional derivatives and some will be exposed below. The comparison between these definitions and their properties will be in this chapter, but it is necessary to introduce some important functions first.

3.1. Important Functions

The Euler Gamma Function, being a generalization of the factorial for real or even complex numbers, is utterly relevant in the posterior definitions.

Definition 3.1.1. *The Euler Gamma function, Γ, is given by*

$$\Gamma(z) = \int_0^\infty x^{z-1}e^{-x}dx, z \in \mathbb{C}. \tag{3-1}$$

As we just mentioned this has a clear relation with factorial. Given $n \in \mathbb{Z}$, then

$$n! = \Gamma(n-1). \tag{3-2}$$

The exponential function has wide importance in the calculus and the differential equations in general, the Mittag-Leffler function is a generalization of it and it is very useful when dealing with fractional derivatives.

Definition 3.1.2. *A two parameter function of the Mittag-Leffler type is defined by*

$$E_{\alpha,\beta}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + \beta)}, \tag{3-3}$$

where $\alpha > 0$, $\beta > 0$ are real constants and Γ is the Gamma function defined by (3-1).

3.2. Fractional Derivatives

The goal in this section is to make sense of non integer orders of differentiation. For this we will start pointing at some formulations made in [38].
The derivative of a function with suitable properties is defined as

$$f'(t) = \lim_{h\to 0} \frac{f(t+h) - f(t)}{h}, \tag{3-4}$$

and similarly

$$f''(t) = \lim_{h\to 0} \frac{f'(t+h) - f'(t)}{h} \tag{3-5}$$

$$= \lim_{h\to 0} \frac{f(t+h) - 2f(t) + f(t-h)}{h^2}. \tag{3-6}$$

Continuing with this idea we can get

$$f^{(n)}(t) = \lim_{h\to 0} \frac{1}{h^n} \sum_{r=0}^{n} (-1)^r \binom{n}{r} f(t - rh), \tag{3-7}$$

where

$$\binom{n}{r} = \frac{n(n-1)(n-2)\cdots(n-r+1)}{r!}. \tag{3-8}$$

Generalizing these formulations, let us define

$$f_h^{(p)}(t) = \frac{1}{h^p} \sum_{r=0}^{n} (-1)^r \binom{p}{r} f(t - rh), \tag{3-9}$$

for $p, n \in \mathbb{Z}$. If $p \leq n$, then

$$\lim_{h\to 0} f_h^{(p)}(t) = f^{(p)}(t). \tag{3-10}$$

We generalize the combinatorial operator as follow

$$\begin{bmatrix} p \\ r \end{bmatrix} = \frac{p(p+1)\cdots(p+r-1)}{r!}, \tag{3-11}$$

which is available for negative integers and real numbers in general:

$$\binom{-p}{r} = \frac{-p(-p-1)\cdots(-p-r+1)}{r!} = (-1)^r \begin{bmatrix} p \\ r \end{bmatrix}. \tag{3-12}$$

Then, we expand the definition of $f_h^{(.)}$

$$f_h^{(-p)}(t) = \frac{1}{h^p} \sum_{r=0}^{n} (-1)^r \begin{bmatrix} p \\ r \end{bmatrix} f(t - rh). \tag{3-13}$$

Taking $h = \frac{t-a}{n}$, where $a \in \mathbb{R}$ is the "initial point", a constant. Then, we establish the next definition as the limit.

Definition 3.2.1. *For a function u, its Grünwald-Letnikov derivative of order α is defined by*

$$
\begin{aligned}
{}_a^{GL}D_t^{\alpha}f(t) &= \lim_{\substack{h\to 0\\ nh=t-a}} f_h^{(\alpha)}(t) && \text{(3-14)}\\
&= \lim_{\substack{h\to 0\\ nh=t-a}} \frac{1}{h^{\alpha}}\sum_{r=0}^{n}(-1)^r\begin{bmatrix}\alpha\\ r\end{bmatrix} f(t-rh) && \text{(3-15)}
\end{aligned}
$$

From this definition, we can perform the special case $\alpha = -1$

$$
\begin{aligned}
{}_a^{GL}D_t^{-1}f(t) &= \lim_{\substack{h\to 0\\ nh=t-a}} f_h^{(-1)}(t) = \lim_{n\to\infty}\frac{1}{h}\sum_{r=0}^{n} f(t-rh) && \text{(3-16)}\\
&= \int_a^t f(\tau)d\tau. && \text{(3-17)}
\end{aligned}
$$

Similarly, if $\alpha = -2$

$$
{}_a^{GL}D_t^{-2}f(t) = \int_a^t (t-\tau)f(\tau)d\tau. \qquad \text{(3-18)}
$$

For a positive integer p, the Cauchy's Integral Rule, which can be proved through repeated integrations by parts, is given by

$$
\frac{1}{(p-1)!}\int_a^t (t-\tau)^{p-1}f(\tau)d\tau = \underbrace{\int_a^t\left(\int_a^t \ldots\left(\int_a^t f(t)dt\right)\ldots dt\right)dt}_{p \text{ times}}. \qquad \text{(3-19)}
$$

Applying Theorem 2.1 from [38], we can conclude that for $p \in \mathbb{R}^+$

$$
{}_a^{GL}D_t^{-p}f(t) = \frac{1}{\Gamma(p)}\int_a^t (t-\tau)^{p-1}f(\tau)d\tau \qquad \text{(3-20)}
$$

Given these facts, we make the next definition.

Definition 3.2.2. *For a function u its Riemann-Liouville derivative of order α is defined by*

$$
{}_a^{RL}Du_t^{(\alpha)}(t) := \frac{1}{\Gamma(n-\alpha)}\frac{d^n}{dt^n}\int_0^t (t-\xi)^{n-1-\alpha}u(\xi)\,d\xi, \quad n-1 \le \alpha < n. \qquad \text{(3-21)}
$$

This derivative has been widely studied through the view of the pure mathematics, but advances in material science requires an update for a better description of the physical properties. Also, the rheological models involve fractional differential equations and the initial conditions need to be formulated properly in a interpretable way. In fractional differential equations with Riemann-Liouville derivatives, the initial conditions must be in the form

$$\lim_{t\to a} u_t(t)^{\alpha-1} = b_1, \tag{3-22}$$
$$\lim_{t\to a} u_t(t)^{\alpha-2} = b_2, \tag{3-23}$$
$$\dots, \tag{3-24}$$
$$\lim_{t\to a} u_t(t)^{\alpha-n} = b_n, \tag{3-25}$$

But for physical problems another initial conditions are required and these often take the form $f(0)$, $f'(0)$, etc. Fortunately, the Caputo definition of fractional derivatives gives an applicable approach.

Definition 3.2.3. *For a function u its Caputo derivative of order α is defined by*

$$u_t^{(\alpha)}(t) := \begin{cases} \dfrac{1}{\Gamma(n-\alpha)} \displaystyle\int_0^t \frac{u^{(n)}(\xi)}{(t-\xi)^{\alpha+1-n}}\, d\xi, & n-1 < \alpha < n, \\ u^{(n)}(t), & \alpha = n, \end{cases} \tag{3-26}$$

with $n \in \mathbb{Z}^+$ and u with at least n derivatives.

3.3. The Laplace and Fourier Transforms of Fractional Derivatives

3.3.1. Laplace Transform

Definition 3.3.1. *A function f is said to be of exponential order γ, if there exist positive constants M and T such that*

$$e^{-\gamma t}|f(t)| \le M, \quad \textit{for all } t > T. \tag{3-27}$$

That is function f does not grow faster than a certain exponential function as $t \to \infty$.

Definition 3.3.2. *Let $f : [0, \infty) \to \mathbb{R}$ a function of exponential order γ, its Laplace transform, $F(s)$, with $s \in \mathbb{C}$, is defined by*

$$F(s) = \mathcal{L}\{f(t); s\} = \int_0^\infty e^{-st} f(t) dt, \tag{3-28}$$

as long as this integral exists.
The function $f(t)$ can be restored from $F(s)$ as follow

$$f(t) = \mathcal{L}^{-1}\{F(s); t\} = \int_{c-i\infty}^{c+i\infty} e^{st} F(s) ds, \qquad c = Re(s) > c_0, \tag{3-29}$$

where $c_0 \in \mathbb{R}$ is in the right half plane of the absolute convergence set, which is the subset of $\mathbb{C}$ where the integral below exists

$$\int_0^\infty |e^{-st} f(t)| dt. \tag{3-30}$$

Remark. *For the functions f and g and assuming its respective Laplace transforms F and G exist, we get*

$$\mathcal{L}\left\{f(t) * g(t); s\right\} = F(s)G(s). \tag{3-31}$$

The next property of the Laplace transform for the derivative of integer order will be needed

$$\mathcal{L}\left\{f^{(n)}(t); s\right\} = s^n F(s) - \sum_{k=0}^{n-1} s^{n-k-1} f^{(k)}(0). \tag{3-32}$$

Let $\alpha \in (0,1)$, then for $t \in \mathbb{R}$ the Laplace transform

$$\mathcal{L}\{t^\alpha; s\} = \int_0^\infty t^\alpha e^{-st} dt \tag{3-33}$$

$$= \frac{\Gamma(\alpha+1)}{s^{\alpha+1}}, \tag{3-34}$$

and this implies that

$$\mathcal{L}\left\{\frac{t^{\alpha-1}}{\Gamma(\alpha)}; s\right\} = \frac{1}{s^\alpha}. \tag{3-35}$$

Theorem 3.3.3. *Under suitable conditions and $n-1 < \alpha < n$*

$$\mathcal{L}\left\{f_t^{(\alpha)}(t); s\right\} = s^\alpha F(s) - \sum_{k=0}^{n-1} s^{\alpha-k-1} f^{(k)}(0). \tag{3-36}$$

Proof.

$$f_t^{(\alpha)}(t) = \frac{1}{\Gamma(n-\alpha)} \int_0^t \frac{f^{(n)}(\xi)}{(t-\xi)^{\alpha+1-n}} d\xi \tag{3-37}$$

$$= \int_0^t f^{(n)}(\xi) \cdot \frac{(t-\xi)^{(n-\alpha)-1}}{\Gamma(n-\alpha)} d\xi \tag{3-38}$$

$$= \left(f^{(n)}(\xi) * \frac{\xi^{(n-\alpha)-1}}{\Gamma(n-\alpha)}\right)(t) \tag{3-39}$$

Now,

$$\begin{aligned}
\mathcal{L}\left\{f_t^{(\alpha)}(t);s\right\} &= \mathcal{L}\left\{\left(f^{(n)}(\xi) * \frac{\xi^{(n-\alpha)-1}}{\Gamma(n-\alpha)}\right)(t);s\right\} && \text{(3-40)}\\
&= \mathcal{L}\left\{\frac{t^{(n-\alpha)-1}}{\Gamma(n-\alpha)};s\right\} \cdot \mathcal{L}\left\{f^{(n)}(t);s\right\} && \text{(3-41)}\\
&= s^{-(n-\alpha)} \cdot \left(s^n F(s) - \sum_{k=0}^{n-1} s^{n-k-1} f^{(k)}(0)\right) && \text{(3-42)}\\
&= s^{\alpha} \cdot F(s) - \sum_{k=0}^{n-1} s^{\alpha-k-1} f^{(k)}(0). && \text{(3-43)}
\end{aligned}$$

□

3.3.2. Fourier Transform

Given a real function $h(t) \in \mathcal{L}^2(\mathbb{R})$ we define its Fourier transform as follow

$$\mathcal{F}\{h(t);\eta\} := \int_{\mathbb{R}} e^{i\eta t} h(t)dt. \tag{3-44}$$

This transform has an inverse, and naming $H(\eta) = \mathcal{F}\{h(t);\eta\}$ applying the Fourier transform in this problem to the variables y and t we get

$$\begin{aligned}
h(t) &:= \frac{1}{2\pi}\int_{\mathbb{R}} e^{-i\eta t} h(t)d\eta && \text{(3-45)}\\
&= \mathcal{F}^{-1}\{H(\eta);t\}. && \text{(3-46)}
\end{aligned}$$

Remark. *For this definition of Fourier transform, if $h(t) \in \mathbb{H}^n(\mathbb{R})$, then*

$$\mathcal{F}\left\{h^{(n)}(t);\eta\right\} = (i\eta)^n H(\eta), \tag{3-47}$$

with $\mathbb{H}^n(\mathbb{R}) := \left\{f \in \mathcal{L}^2(\mathbb{R}) : \sum_{k=0}^{n} \|f^{(k)}\|_2^2\right\}$.

Replacing $s = i\eta$ in 3-35 and defining $h(t)$ to be

$$h(t) = \begin{cases} \frac{t^{\alpha-1}}{\Gamma(\alpha)}, & t > 0 \\ 0, & t \le 0 \end{cases} \tag{3-48}$$

then

$$\begin{aligned}
\mathcal{F}\{h(t);\eta\} &= \int_{\mathbb{R}} e^{i\eta t} h(t)dt = \int_0^{\infty} e^{-st}\frac{t^{\alpha-1}}{\Gamma(\alpha)}dt = s^{-\alpha} && \text{(3-49)}\\
&= (i\eta)^{-\alpha}. && \text{(3-50)}
\end{aligned}$$

Now, given a function $g \in \mathcal{L}^2(\mathbb{R})$ then

$$\mathcal{F}\{h(t) * g(t); \eta\} = (i\eta)^\alpha G(\eta), \tag{3-51}$$

Since we established this behavior of the Fourier Transform, for a function $g \in \mathbb{H}^n(\mathbb{R})$ its Caputo derivative of order $\alpha \in (n-1, n)$

$$\begin{aligned} g_t^{(\alpha)}(t) &= \frac{1}{\Gamma(n-\alpha)} \int_0^t \frac{g^{(n)}(\xi)}{(t-\xi)^{\alpha+1-n}}\, d\xi && \text{(3-52)} \\ &= \int_0^t g^{(n)}(\xi) \cdot \frac{(t-\xi)^{(n-\alpha)-1}}{\Gamma(n-\alpha)}\, d\xi && \text{(3-53)} \\ &= \left(g^{(n)}(\xi) * \frac{\xi^{(n-\alpha)-1}}{\Gamma(n-\alpha)} \right)(t) && \text{(3-54)} \end{aligned}$$

and taking Fourier Transform,

$$\begin{aligned} \mathcal{F}\left\{ g_t^{(\alpha)}(t); \eta \right\} &= \mathcal{F}\left\{ \left(g^{(n)}(\xi) * \frac{\xi^{(n-\alpha)-1}}{\Gamma(n-\alpha)} \right)(t); \eta \right\} && \text{(3-55)} \\ &= (i\eta)^{\alpha-n} \cdot \mathcal{F}\left\{ g^{(n)}(\xi); \eta \right\} && \text{(3-56)} \\ &= (i\eta)^{\alpha-n} \cdot (i\eta)^n \cdot G(\eta) && \text{(3-57)} \\ &= (i\eta)^\alpha \cdot G(\eta) && \text{(3-58)} \end{aligned}$$

3.4. Existence and Uniqueness Theorems

Lets consider the next initial-value problem:

$$\begin{cases} u_t^{(\alpha)}(t) + \sum_{m=1}^n p_{n-m}(t) u_t^{(m-1)} = f(t), & 0 < t < T < \infty \\ u(0) = b_0, \\ u_t^{(1)}(0) = b_1, \\ \dots, \\ u_t^{(n-1)}(0) = b_{n-1}, \end{cases} \tag{3-59}$$

where $n - 1 < \alpha < n$ and

$$\int_0^T |f(t)| dt < \infty. \tag{3-60}$$

Theorem 3.4.1. *If $f(t) \in \mathcal{L}_1(0,T)$, then the equation*

$$u_t^{(\alpha)}(t) = f(t) \tag{3-61}$$

has a unique solution $u(t) \in \mathcal{L}_1(0,T)$, which satisfies the initial conditions 3-59.

Proof. We will apply Laplace transform in both sides of the differential equation

$$s^{\alpha}U(s) - \sum_{k=0}^{n-1} s^{\alpha-k-1} b_k = F(s) \tag{3-62}$$

where $U(s)$ and $F(s)$ are the Laplace transforms of $u(t)$ and $f(t)$ respectively. Resolving for $U(s)$

$$U(s) = s^{-\alpha}F(s) + \sum_{k=0}^{n-1} s^{-k-1} b_k \tag{3-63}$$

and the inverse Laplace gives

$$u(t) = \frac{1}{\Gamma(\alpha)} \int_0^t (t-\eta)^{\alpha-1} f(\eta) d\eta + \sum_{k=0}^{n-1} \frac{b_k}{\Gamma(k+1)} t^k. \tag{3-64}$$

From this equation, we conclude $u(t) \in \mathcal{L}_1(0,T)$. Now, if there were two solutions $u_1(t)$ and $u_2(t)$ of the problem (3-59), then if $z(t) = u_1(t) - u_2(t)$, this is a solution of the equation $z_t^{(\alpha)}(t) = 0$ and zero initial conditions. This last statement implies $Z(s) = 0$, and good properties of the Laplace transform gives us $z(t) = 0$ almost everywhere, which proves the solution is unique in $\mathcal{L}_1(0,T)$. □

Theorem 3.4.2. *If $f(t) \in \mathcal{L}_1(0,T)$, and $p_m(t)$, $m = 1, \ldots n$ are continuous functions in the closed interval $[0,T]$, then the initial-value problem (3-59) has a unique solution $u(t) \in \mathcal{L}_1(0,T)$.*

Proof. This proof follows the one in [38] modified for Caputo derivative. Lets assume 3-59 has a solution $u(t)$ and denote

$$u_t^{(\alpha)}(t) = \phi(t). \tag{3-65}$$

As a consequence of (3.4.1)

$$u(t) = \frac{1}{\Gamma(\alpha)} \int_0^t (t-\eta)^{\alpha-1} \phi(t) dt + \sum_{k=0}^{n-1} \frac{b_k}{\Gamma(k+1)} t^k. \tag{3-66}$$

Substituting this in the differential equation, we obtain the equation

$$\phi(t) + \int_0^t K(t,\tau)\phi(\tau) d\tau = g(t), \tag{3-67}$$

where

$$K(t,\tau) = \sum_{m=1}^{n} p_{n-m}(t) \frac{(t-\tau)^{m-1}}{\Gamma(m)}, \tag{3-68}$$

$$g(t) = f(t) - \sum_{m=1}^{n} \frac{b_{m-1}}{\Gamma(m)} t^{m-1}. \tag{3-69}$$

The continuity of the functions $p_j(t)$, $j = 1, \ldots, n$ implies that the kernel $K(t, \tau)$ is also continuous for $0 \leq t \leq T$, $0 \leq \tau \leq T$. Similarly $g(t)$ is continuous in $[0, T]$, and that implies there exist $\phi(t) \in \mathcal{L}_1(0, T)$ the unique solution of (3-67) (Theorem 3.1 from [26]), therefore, since Theorem 3.4.1, we can conclude $u(t)$ exists and it is the unique solution for (3-59). □

3.5. An Application of Fractional Calculus

To end this chapter, we show an application that can be found in the book of Diethelm ([15]). In mechanics the behavior of a solid in a stress setting is modeled by Hooke's Law which relates the stress σ and the strain ε. This is given by

$$\sigma(t) = E\varepsilon(t), \tag{3-70}$$

being both functions of the time t and the number E is called the elasticity modulus.
For viscous liquids the Newton's Law gives us a similar formulation between these quantities, namely

$$\sigma(t) = \eta D^1\varepsilon(t). \tag{3-71}$$

The constant η is the viscosity of the material. For convenience, we can rewrite Hooke's Law as follow

$$\sigma(t) = ED^0\varepsilon(t). \tag{3-72}$$

The appearance of materials that behave in "between" the solid and the viscous way, arose to the model of Nutting ([35], [36]) derivatives play a fundamental role. This "interpolation" takes the form

$$\sigma(t) = \nu D^\alpha\varepsilon(t), \tag{3-73}$$

with $0 < \alpha < 1$ and ν is a material constant. This approach is comonly called the *Nutting's Law*. The work of Scott Blair and Reiner [42] confirms the practical importance of this model.
This chapter and chapter 2 introduce preliminary definitions and results of importance for the thesis. The first interactions between inverse problems and fractional differential equations appear in the next chapter.

4. Fractional Diffusion Equation and Source Term Identification

In the first part of this chapter we consider a two-dimensional time fractional diffusion equation and address the important inverse problem consisting on the identification of a space dependent factor in the source term. The fractional derivative is in the sense of Caputo. The necessary regularization procedure is provided by a two-dimensional discrete mollification operator. Convergence results and illustrative numerical examples are included. For this part we follow [16] closely. The second part of the chapter deals with the same two dimensional time fractional differential equation with time derivative in the sense of Caputo. The inverse problem consists on the recovery of a time dependent factor in the source term. Error estimates and numerical examples are included. We begin with some theoretical results.

4.1. Preliminaries

The Sobolev Space $W^{k,p}(\Omega)$ (as is defined in [18]), with $p \geq 1$ and $k \in \mathbb{Z}^+$, is given by

$$W^{k,p}(\Omega) = \left\{ u \in W^k(\Omega); D^\beta u \in L^p(\Omega) \text{ for all multi-index } \beta : |\beta| \leq k \right\}.$$

Here D^β represents the derivatives operator $D^\beta u = \frac{\partial^k u}{\partial x_1^{\beta_1} \partial x_2^{\beta_2} \cdots \partial x_n^{\beta_n}}$. In this space the norm would be

$$\|u\|_{W^{k,p}(\Omega)} = \left(\int_\Omega \sum_{|\beta| \leq k} |D^\beta u|^p \right)^{1/p}.$$

Some of these sets are important for the next analysis and are established in Brezis [12] and Salsa [41]. For $1 \leq p < \infty$, the closure of $C_c^1(\Omega)$ in $W^{1,p}$ is denoted by $W_0^{1,p}$. Moreover, we set

$$H_0^1(\Omega) = W_0^{1,2},$$
$$H^2 = \left\{ u \in L^2(\Omega) : D^\beta u \in L^2(\Omega), \text{ for all multi-index } \beta : |\beta| \leq 2 \right\}.$$

We are particularly interested in the *Uniformly Symmetric Elliptic Operator* $-L$ defined below as in [18] and [40]

$$Lu(z) = \sum_{i=1}^{d} \frac{\partial}{\partial z_i}\left(\sum_{j=1}^{d} a_{ij}(z)\frac{\partial}{\partial z_j}u(z)\right) + c(z)u(z), z \in \Omega. \tag{4-1}$$

The coefficients satisfy $a_{ij} = a_{ji} \in C^1(\bar{\Omega})$, $\sum_{i,j=1}^{d} a_{ij}\zeta_i\zeta_j > \theta \sum_{i=1}^{d} |\zeta_i|^2$ ($\theta > 0$), $c(z) \leq 0$, $c \in C(\bar{\Omega})$. With these conditions $-L$ is a symmetric uniformly elliptic operator defined on $D(-L) = H^2(\Omega) \cap H_0^1(\Omega)$. The eigenfunctions and eigenvalues of $-L$ are denoted by $\{\chi_n\}_{n\in\mathbb{N}}$ and $\{\lambda_n\}_{n\in\mathbb{N}}$, respectively. As in [40], $(-L)^\gamma$ is defined for $\gamma \in \mathbb{R}$ and the space

$$D\left((-L)^\gamma\right) = \left\{\psi \in L^2(\Omega) : \sum_{n=1}^{\infty} \lambda_n^{2\gamma}|(\psi, \chi_n)|^2 < \infty\right\}, \tag{4-2}$$

where $(\cdot, \cdot)$ is the inner product in $L^2(\Omega)$, becomes a Hilbert space with the norm

$$\|\psi\|_{D((-L)^\gamma)} = \left(\sum_{n=1}^{\infty} \lambda_n^{2\gamma}|(\psi, \chi_n)|^2\right)^{\frac{1}{2}}. \tag{4-3}$$

The eigenvalues and eigenfunctions of operator $-L$ will be used for solving the direct and inverse problems based on the following set of equations.

$$\left.\begin{array}{llll} D_t^\alpha u(z,t) - (Lu)(z,t) & = F(z,t), & z \in \Omega & t \in (0,T) \\ u(z,t) & = 0, & z \in \partial\Omega & t \in (0,T) \\ u(z,0) & = 0, & z \in \bar{\Omega} & \end{array}\right\} \tag{4-4}$$

In Sakamoto-Yamamoto [40] the solution for this problem is given by

$$u(x,t) = \sum_{n=1}^{\infty} \left(\int_0^t \langle F(\cdot,\tau), \chi_n\rangle (t-\tau)^{\alpha-1} E_{\alpha,\alpha}\left(-\lambda_n(t-\tau)^\alpha\right) d\tau\right) \chi_n(x),$$

if $F \in L^\infty(0,T; L^2(\Omega))$.

4.2. Space dependent factor of the source term

We are interested in an initial/boundary value problem in which the time derivative is a Caputo fractional derivative of order α, $0 < \alpha < 1$.
In this section we introduce the theoretical setting for an identification problem based on the following initial/boundary value problem:

$$\left.\begin{array}{llll} D_t^\alpha u(z,t) - (Lu)(z,t) & = p(t)f(z), & z \in \Omega & t \in (0,T) \\ u(z,t) & = 0, & z \in \partial\Omega & t \in (0,T) \\ u(z,0) & = 0, & z \in \bar{\Omega} & \end{array}\right\} \tag{4-5}$$

where $\Omega \subset \mathbb{R}^d$.
The identification problem based on (4-5) is:

$$\begin{array}{lrr} p(t) & & \text{known.} \\ u(z,T) = q(z), & z \in \mathring{\Omega} & \text{known.} \\ a,b,c,d & \text{defined on } \Omega \times [0,T] & \text{known.} \\ u(z,0) = 0, & z \in \Omega & \text{known.} \\ u(z,t) = 0, & (z,t) \in \partial\Omega \times (0,T] & \text{known.} \\ f(z) & z \in \Omega & \text{unknown.} \\ u(z,t), & (z,t) \in \mathring{\Omega} \times (0,T) & \text{unknown.} \end{array}$$

Here $\mathring{\Omega}$ means the interior of the domain Ω. Since we are dealing with an inverse problem, some overposed data is mandatory. In our case the overposed data is a future time value of the concentration u given by $u(z,T) = q(z)$. However, we do not know q exactly, there is a noise level ϵ and a noisy version of q, denoted q^ϵ, satisfying $\|q - q^\epsilon\|_\infty < \epsilon$.

As in [40] and [28] it is possible to obtain a solution for the direct problem (1-6) in the following form:

$$u(z,t) = \sum_{n=1}^{\infty} f_n \int_0^t p(\tau)\,(t-\tau)^{\alpha-1}\, E_{\alpha,\alpha}\left(-\lambda_n\,(t-\tau)^{\alpha}\right) d\tau \chi_n(z). \tag{4-6}$$

where $f_n = \langle f, \chi_n \rangle$. Hence,

$$\begin{aligned} u(z,T) &= \sum_{n=1}^{\infty} f_n \int_0^T p(\tau)\,(T-\tau)^{\alpha-1}\, E_{\alpha,\alpha}\left(-\lambda_n\,(T-\tau)^{\alpha}\right) d\tau \chi_n(z), & \text{(4-7)} \\ &= q(z). & \text{(4-8)} \end{aligned}$$

Setting

$$Q_n(t) = \int_0^t p(\tau)\,(t-\tau)^{\alpha-1}\, E_{\alpha,\alpha}\left(-\lambda_n\,(t-\tau)^{\alpha}\right) d\tau, \tag{4-9}$$

with

$$E_{\alpha,\alpha} = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + \alpha)}.$$

Thus,

$$q(z) \;=\; \sum_{n=1}^{\infty} f_n Q_n(T) \chi_n(z), \tag{4-10}$$

and its Fourier coefficients are $q_n = f_n Q_n(T)$. We conclude $f_n = \dfrac{q_n}{Q_n(T)}$.

4.2.1. Mollified Problem

The ill-posing of the classical diffusion problem ($\alpha = 1$) is exposed in [24]. Now, if q_ϵ is a noisy version of the exact data q such that $\|q^\epsilon - q\| \leq \epsilon$, the convergence of $q_n^\epsilon / Q_n(T)$ cannot be ensured. We propose a mollified version of the problem as follows

$$\begin{array}{lrr}
J_{\delta\eta} p(t) & & \text{known.} \\
J_{\delta\eta} u(z,T) = J_{\delta\eta} q(z), & z \in \mathring{\Omega} & \text{known.} \\
a, b, c, d & \text{defined on } \Omega \times [0,T] & \text{known.} \\
J_{\delta\eta} u(z,0) = 0, & z \in \Omega & \text{known.} \\
J_{\delta\eta} u(z,t) = 0, & (z,t) \in \partial\Omega \times (0,T] & \text{known.} \\
J_{\delta\eta} f(z) & z \in \Omega & \text{unknown.} \\
J_{\delta\eta} u(z,t), & (z,t) \in \mathring{\Omega} \times (0,T) & \text{unknown.}
\end{array}$$

We can formulate our problem in the framework of optimization. First, we define the operator

$$(Kf)(z) \quad = \quad \sum_{n=1}^{\infty} f_n \int_0^t p(\tau)\,(t-\tau)^{\alpha-1} E_{\alpha,\alpha}\left(-\lambda_n (t-\tau)^{\alpha}\right) d\tau \chi_n(z), \tag{4-11}$$

then, our aim is to obtain a function f_δ^ϵ that minimizes the functional

$$Hf = \|Kf - J_{\delta\eta} q^\epsilon\|_2^2, \tag{4-12}$$

where $J_{\delta p} q^\epsilon$ is the mollification of the noisy data q^ϵ.

Since K is a self-adjoint compact operator as is mentioned in [28], there exists a minimum of H, f_δ^ϵ, given by

$$f_\delta^\epsilon(z) = \sum_{n=1}^{\infty} \frac{\left(J_{\delta\eta} q^\epsilon\right)_n}{Q_{n(T)}} \chi_n(z), \quad \textit{where} \quad \left(J_{\delta\eta} q^\epsilon\right)_n = \left\langle J_{\delta\eta} q^\epsilon, \chi_n \right\rangle. \tag{4-13}$$

Theorem 4.2.1. *Suppose* $p \in C[0,T]$ *satisfies* $p(t) \geq p_0 > 0, t \in [0,T]$. *Moreover, suppose* $\|q^\epsilon - q\|_\infty < \epsilon$ *and there exist* $m \in \mathbb{R}^+$ *and* E *a constant such that* $\|f\|_{\mathcal{D}((-L)^{\frac{m}{2}})} \leq E$ *then*

$$\|f_\delta^\epsilon - f\|_2 \leq C_1 \left(\delta + \epsilon\right)^{m/(m+2)}, \tag{4-14}$$

where C_1 *depends on* α, T, λ_1 *and the measure of* Ω.

Proof.

$$\|f_\delta^\epsilon\|^2_{\mathcal{D}((-L)^{\frac{m}{2}})} = \left|\sum_{n=1}^{\infty}\lambda_n^m (f_\delta^\epsilon, \chi_n(z))^2\right| \tag{4-15}$$

$$= \left|\sum_{n=1}^{\infty}\lambda_n^m (f_\delta^\epsilon)_n^2\right| \tag{4-16}$$

$$= \left|\sum_{n=1}^{\infty}\lambda_n^m \frac{(J_{\delta\eta}q^\epsilon)_n^2}{Q^2_{n(T)}}\right| \tag{4-17}$$

$$\leq \left|\sum_{n=1}^{\infty}\frac{\lambda_n^{m+2}}{\underline{C}^2 p_0^2}(J_{\delta\eta}q^\epsilon, \chi_n(z))^2\right| \tag{4-18}$$

$$= \frac{1}{\underline{C}^2 p_0^2}\left|\sum_{n=1}^{\infty}\lambda_n^{m+2}(J_{\delta\eta}q^\epsilon, \chi_n(x,y))^2\right| \tag{4-19}$$

$$= \frac{1}{\underline{C}^2 p_0^2}\|J_{\delta\eta}q^\epsilon\|^2_{\mathcal{D}((-L)^{\frac{m}{2}+1})}. \tag{4-20}$$

But $J_{\delta\eta}q^\epsilon \in C^\infty(\Omega)$, which implies $f_\delta^\epsilon \in \mathcal{D}((-L)^{\frac{m}{2}})$. Taking $M = \max\{\|J_{\delta\eta}q^\epsilon\|_{\mathcal{D}((-L)^{\frac{m}{2}+1})}, E\}$, we obtain

$$\|Kf_\delta^\epsilon - q\|_2 \leq \|Kf_\delta^\epsilon - J_{\delta\eta}q^\epsilon\|_2 + \|J_{\delta\eta}q^\epsilon - q\|_2 \tag{4-21}$$

$$\leq \|Kf - J_{\delta\eta}q^\epsilon\|_2 + \|J_{\delta\eta}q^\epsilon - q\|_2 = 2\|J_{\delta\eta}q^\epsilon - q\|_2 \tag{4-22}$$

$$\leq C(\delta+\epsilon). \tag{4-23}$$

$$\|f_\delta^\epsilon - f\|_{\mathcal{D}((-L)^{m/2})} \leq |f_\delta^\epsilon\|_{\mathcal{D}((-L)^{m/2})} + \|f\|_{\mathcal{D}((-L)^{m/2})} \tag{4-24}$$

$$\leq M\left(1+\frac{1}{\underline{C}p_0}\right). \tag{4-25}$$

From last two inequalities we conclude that

$$\|f_\delta^\epsilon - f\|_2 \leq (\underline{C}p_0)^{-\frac{m}{m+2}}\|Kf_\delta^\epsilon - q\|_2^{m/(m+2)}\|f_\delta^\epsilon - f\|^{2/(m+2)}_{\mathcal{D}((-L)^{m/2})} \tag{4-26}$$

$$\leq (\underline{C}p_0)^{-\frac{m}{m+2}}\left(M\left(1+\frac{1}{\underline{C}p_0}\right)\right)^{2/(m+2)}(C(\delta+\epsilon))^{m/(m+2)}. \tag{4-27}$$

□

This theorem establishes the convergence of the method.

4.2.2. Results

Numerical results for the identification of $f(z)$ in the following time fractional diffusion problem are shown in this section.

$$\left.\begin{array}{llll} D_t^\alpha u(z,t) - (Lu)(z,t) & = p(t)f(z), & z\in\Omega & t\in(0,T) \\ u(z,t) & = 0, & z\in\partial\Omega & t\in(0,T) \\ u(z,0) & = 0, & z\in\bar{\Omega} & t\in(0,T) \end{array}\right\} \tag{4-28}$$

where,

$$Lu(x,y) = \frac{\partial}{\partial x}\left(a_{11}(x,y)\frac{\partial}{\partial x}u(x,y)\right) + \frac{\partial}{\partial y}\left(a_{22}(x,y)\frac{\partial}{\partial y}u(x,y)\right). \tag{4-29}$$

The equation is discretized by the implicit finite difference scheme which is elaborated in detail in [32]. The operator L is decomposed by its eigenvectors and eigenvalues and the Q_n's are approximated by [28]

$$Q_n = -\frac{1}{\lambda_n}\left(E_{\alpha,1}(-\lambda_n\tau^\alpha)p(T-\tau)\Big|_{\tau=T} - p(T-t)\Big|_{\tau=0} - \int_0^T E_{\alpha,1}(-\lambda_n\tau^\alpha)p'(T-\tau)d\tau\right). \tag{4-30}$$

The integral above is approximated by composite trapezoidal rule.
The errors are measured by the weighted discrete l_2 norm given by

$$\|f - f_\delta^\epsilon\|_2 \;=\; \left(\frac{1}{NM}\sum_{n=1}^{N}\sum_{m=1}^{M}(f_{nm} - (f_\delta^\epsilon)_{nm})^2\right)^{1/2}. \tag{4-31}$$

Where N and M are the grid sizes in the discretization of Ω.
The particular examples considered here are for:

$$f(x,y) \;=\; sin(3\pi x)sin(3\pi y) \tag{4-32}$$
$$p(t) \;=\; 1 + exp(-(t+\alpha)) \tag{4-33}$$

For the following examples, we use the same step sizes for x and y, $h = 1/32$, our final time is $T = 1$ and $\Delta t = 1/10$.

Example 4.2.2. Let $a_{11}(x,y) = x^2 + 1, a_{22}(x,y) = y^2 + 1$. First of all, we compute without mollification. Table **4-1** indicates the ill-posedness of the problem and the need of a regularization method.

Table 4-1.: Error norms without mollification, $\alpha = 0.7$.

ϵ	error
0,005	0,100268
0,01	0,192743
0,025	0,496786
0,05	0,496786

The error norm 4-31 of some identification experiments are shown in Tables **4-2** and **4-3** and in figure **4-1**

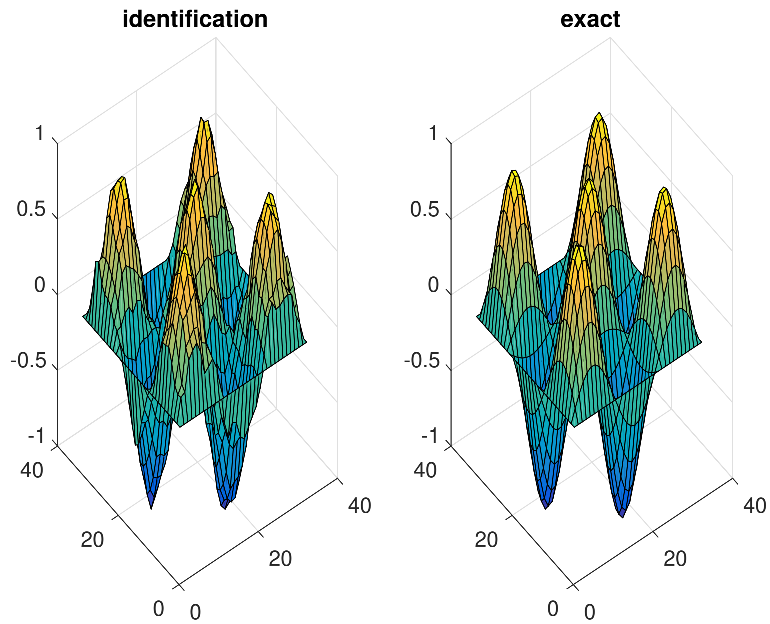

Figure 4-1.: Comparison between the approximation and the exact solution for $h = 1/32$, $\eta = 3$

Table 4-2.: Error norms, $\epsilon = 0.025$ and different values of η and α.

$\alpha\backslash\eta$	1	2	3	4
0,1	0,296105	0,114359	0,073857	0,096831
0,5	0,292845	0,119839	0,078034	0,096871
0,7	0,289358	0,116701	0,075705	0,097454
0,9	0,289503	0,118838	0,079958	0,101561

Table 4-3.: Error norms, $\alpha = 0.7$ and different values of η and ϵ.

$\epsilon\backslash\eta$	1	2	3	4
0,005	0,068577	0,045929	0,057815	0,094482
0,01	0,12205	0,060636	0,061464	0,095757
0,025	0,289539	0,12113	0,078236	0,097298
0,05	0,289539	0,12113	0,078236	0,097298

Example 4.2.3. Let $a_{11}(x, y) \equiv 1$ and $a_{22}(x, y) \equiv 1$. Relative l_2 errors for the identification of the source term are shown in Tables 4-4 and 4-5.

Table 4-4.: Error norms, $\epsilon = 0.025$ and different values of η and α.

$\alpha \backslash \eta$	1	2	3	4
0,1	0,215196	0,085461	0,060851	0,091498
0,5	0,222888	0,088172	0,061884	0,092143
0,7	0,230786	0,089855	0,061206	0,091458
0,9	0,223325	0,088232	0,061837	0,092622

Table 4-5.: Error norms, $\alpha = 0.7$ and different values of η and ϵ.

$\epsilon \backslash \eta$	1	2	3	4
0,005	0,045382	0,026522	0,046967	0,089274
0,01	0,090063	0,039821	0,048425	0,089084
0,025	0,219032	0,088232	0,064776	0,095143
0,05	0,43733	0,172126	0,09563	0,104285

As conclusions of our work in this section, we mention the following:

1. The proposed method can approximate the exact solution of this challenging inverse problem.

2. The two dimensional discrete mollification, under an appropriate choosing of η, operator is effective as a regularization method.

Next section deals with a close inverse problem: Identification of the forcing term factor $p(t)$ known as attenuation coefficient.

4.3. Time dependent factor of the source term

In this section we profit from the theoretical developments of last section to solve other challenging inverse problem: The identification of the time dependent factor $p(t)$ of the forcing term in the initial/boundary value problem:

$$\left.\begin{aligned} D_t^\alpha u(z,t) - (Lu)(z,t) &= p(t)f(z), & z \in \Omega, \quad & t \in (0,T) \\ u(z,t) &= 0, & z \in \partial\Omega, \quad & t \in (0,T) \\ u(z,0) &= 0, & z \in \bar{\Omega} \quad & \end{aligned}\right\} \tag{4-34}$$

where $\Omega \subset \mathbb{R}^2$. The discharge magnitude $f(z)$ is known and so is an overposed data consisting on a complete concentration history at an interior point $z_0 \in \Omega$ for any time $t \in [0,T]$.
The solution for the direct problem ([40]) is given by

$$u(z,t) = \sum_{n=1}^{\infty} f_n \int_0^t p(\tau)\,(t-\tau)^{\alpha-1}\, E_{\alpha,\alpha}\left(-\lambda_n\,(t-\tau)^{\alpha}\right) d\tau \chi_n(z), \tag{4-35}$$

where

$$f_n = \langle f, \chi_n \rangle, \;\; n \in \mathbb{N}, \tag{4-36}$$

and $\{(\lambda_n, \chi_n) : n = 1, 2, \ldots\}$ are the eigenvalues and eigenfunctions for the Sturm-Liouville two point boundary problem:

$$\mathcal{L}\chi_n := -\frac{\partial^2}{\partial z^2} = \lambda_n \chi_n, \quad \text{on } (0,1), \quad \chi_n(0) = \chi(1) = 0, \tag{4-37}$$

as is addressed in [44].

4.3.1. Proposed Approximation

In [49] is solved a similar problem with a midpoint quadrature, we will develop a method based on a rectangular quadrature with an exact calculation of the integration of the kernel of this integral equation. First, we make a discretization in the interval $[0, T]$ with grid size $\Delta t = T/M$ and $t_i = i\Delta t$. Naming

$$h_i = u(z_0, t_i), \quad\; i = 1 : M, \tag{4-38}$$

we get

$$h_1 = \sum_{n=1}^{\infty} f_n \int_0^{t_1} p(\tau) \left(t_1 - \tau\right)^{\alpha - 1} E_{\alpha,\alpha} \left(-\lambda_n \left(t_1 - \tau\right)^{\alpha}\right) d\tau \chi_n(z_0). \tag{4-39}$$

The numerical method will approximate the integral following the ideas bellow. If $p(t_1)$ is estimated with P_1, from the equation above the

$$\begin{aligned} h_1 &= \sum_{n=1}^{\infty} f_n \int_0^{t_1} P_1 \left(t_1 - \tau\right)^{\alpha - 1} E_{\alpha,\alpha} \left(-\lambda_n \left(t_1 - \tau\right)^{\alpha}\right) d\tau \chi_n(z_0) &\text{(4-40)} \\ &= \sum_{n=1}^{\infty} f_n P_1 \int_0^{t_1} \left(t_1 - \tau\right)^{\alpha - 1} E_{\alpha,\alpha} \left(-\lambda_n \left(t_1 - \tau\right)^{\alpha}\right) d\tau \chi_n(z_0). &\text{(4-41)} \end{aligned}$$

We concentrate on the integral, namely

$$\begin{aligned} &\int_0^{t_1} \left(t_1 - \tau\right)^{\alpha - 1} E_{\alpha,\alpha} \left(-\lambda_n \left(t_1 - \tau\right)^{\alpha}\right) d\tau \\ &= \int_0^{t_1} \left(t_1 - \tau\right)^{\alpha - 1} \sum_{k=0}^{\infty} \frac{(-\lambda_n)^k \left(t_1 - \tau\right)^{\alpha k}}{\Gamma(\alpha k + \alpha)} d\tau \\ &= \int_0^{t_1} \sum_{k=0}^{\infty} \frac{(-\lambda_n)^k \left(t_1 - \tau\right)^{\alpha k + \alpha - 1}}{\Gamma(\alpha k + \alpha)} d\tau \end{aligned}$$

$$
\begin{aligned}
&= \sum_{k=0}^{\infty} \int_0^{t_1} \frac{(-\lambda_n)^k (t_1-\tau)^{\alpha k+\alpha-1}}{\Gamma(\alpha k+\alpha)} d\tau \\
&= \sum_{k=0}^{\infty} \left(- \frac{(-\lambda_n)^k (t_1-\tau)^{\alpha k+\alpha}}{\Gamma(\alpha k+\alpha)(\alpha k+\alpha)} \right|_{\tau=0}^{\tau=t_1} \\
&= \sum_{k=0}^{\infty} \frac{(-\lambda_n)^k (t_1)^{\alpha k+\alpha}}{\Gamma(\alpha k+(\alpha+1))} \\
&= (t_1)^{\alpha} \sum_{k=0}^{\infty} \frac{(-\lambda_n)^k (t_1)^{\alpha k}}{\Gamma(\alpha k+(\alpha+1))} \\
&= (t_1)^{\alpha} E_{\alpha,\alpha+1}\left(-\lambda_n (t_1)^{\alpha}\right).
\end{aligned}
$$

The integral and the summation can be exchanged because the Mittag-Leffler function is analytic. From above, we get

$$
\begin{aligned}
h_1 &= P_1 \sum_{n=1}^{\infty} f_n (t_1)^{\alpha} E_{\alpha,\alpha+1}\left(-\lambda_n (t_1)^{\alpha}\right) \chi_n(z_0) \\
&= P_1 \sum_{n=1}^{\infty} f_n (\Delta t)^{\alpha} E_{\alpha,\alpha+1}\left(-\lambda_n (\Delta t)^{\alpha}\right) \chi_n(z_0).
\end{aligned} \tag{4-42}
$$

In a similar way, P_2 is defined:

$$
\begin{aligned}
h_2 &= P_2 \sum_{n=1}^{\infty} f_n (t_1)^{\alpha} E_{\alpha,\alpha+1}\left(-\lambda_n (t_1)^{\alpha}\right) \chi_n(z_0) + \\
&\quad P_1 \sum_{n=1}^{\infty} f_n \Big((t_2)^{\alpha} E_{\alpha,\alpha+1}\left(-\lambda_n (t_2)^{\alpha}\right) - (t_1)^{\alpha} E_{\alpha,\alpha+1}\left(-\lambda_n (t_1)^{\alpha}\right) \Big) \chi_n(z_0) \\
&= P_2 \sum_{n=1}^{\infty} f_n (\Delta t)^{\alpha} E_{\alpha,\alpha+1}\left(-\lambda_n (\Delta t)^{\alpha}\right) \chi_n(z_0) + \\
&\quad P_1 \sum_{n=1}^{\infty} f_n \Big((2\Delta t)^{\alpha} E_{\alpha,\alpha+1}\left(-\lambda_n (2\Delta t)^{\alpha}\right) - (\Delta t)^{\alpha} E_{\alpha,\alpha+1}\left(-\lambda_n (\Delta t)^{\alpha}\right) \Big) \chi_n(z_0).
\end{aligned}
$$

In general,

$$
h_m = P_m \sum_{n=1}^{\infty} f_n (\Delta t)^{\alpha} E_{\alpha,\alpha+1}\left(-\lambda_n (\Delta t)^{\alpha}\right) \chi_n(z_0) + \ldots
$$

$$
P_{m-1} \sum_{n=1}^{\infty} f_n \Big((2\Delta t)^{\alpha} E_{\alpha,\alpha+1}\left(-\lambda_n (2\Delta t)^{\alpha}\right) - (\Delta t)^{\alpha} E_{\alpha,\alpha+1}\left(-\lambda_n (\Delta t)^{\alpha}\right) \Big) \chi_n(z_0) + \ldots
$$

$$
P_1 \sum_{n=1}^{\infty} f_n \Big((m\Delta t)^{\alpha} E_{\alpha,\alpha+1}\left(-\lambda_n (m\Delta t)^{\alpha}\right) - ((m-1)\Delta t)^{\alpha} E_{\alpha,\alpha+1}\left(-\lambda_n ((m-1)\Delta t)^{\alpha}\right) \Big) \chi_n(z_0).
$$

Calling

$$a_i = \sum_{n=1}^{\infty} f_n \left((i\Delta t)^\alpha E_{\alpha,\alpha+1} \left(-\lambda_n \left(i\Delta t \right)^\alpha \right) - ((i-1)\Delta t)^\alpha E_{\alpha,\alpha+1} \left(-\lambda_n \left((i-1)\Delta t \right)^\alpha \right) \right) \chi_n(z_0),$$

we can write the problem in matrix form as follows

$$b = AP \tag{4-43}$$

with

$$b = \begin{bmatrix} h_1 \\ h_2 \\ \vdots \\ h_M \end{bmatrix}, \quad A = \begin{bmatrix} a_1 & & & \\ a_2 & a_1 & & \\ \vdots & \vdots & \ddots & \\ a_M & a_{M-1} & \cdots & a_1 \end{bmatrix}, \quad P = \begin{bmatrix} P_1 \\ P_2 \\ \vdots \\ P_M \end{bmatrix}. \tag{4-44}$$

The term $E_{\alpha,\alpha+1}(0) \neq 0$, then the matrix does not get singular when $\Delta t \to 0$.

4.3.2. Theoretical Approach

If $K(s,z) := \sum_{n=1}^{\infty} f_n(s)^{\alpha-1} E_{\alpha,\alpha} \left(-\lambda_n \left(s \right)^\alpha \right) \chi_n(z)$, then

$$u(z,t) = \int_0^t p(\tau) K(t-\tau, z) d\tau, \tag{4-45}$$

which we can write as follow

$$Kp(t) := \int_0^t p(\tau) K(t-\tau, z) d\tau. \tag{4-46}$$

The P sequence defined above becomes

$$P_1 = \frac{h(t_1)}{a_1} \tag{4-47}$$

$$P_2 = \frac{h(t_2)}{a_1} - \frac{a_2 P_1}{a_1} \tag{4-48}$$

$$\dots \tag{4-49}$$

$$P_m = \frac{h(t_m)}{a_1} - \sum_{i=1}^{m-1} \frac{a_{m-i+1} P_i}{a_1} \tag{4-50}$$

The goal is to have convergence of the P sequence to the function p. In the presence of noise, regularization is mandatory. Our selected method is discrete mollification with regularization parameter either δ or η. The maximum level of noise in the data is ϵ.

$J_{\delta\eta}p(t)$		unknown.
$J_{\delta\eta}u(z_0,t) = h(t),$	$z_0 \in \Omega$	known.
$a_{ij}, c,$	defined on $\Omega \times [0,T]$	known.
$J_{\delta\eta}u(z,0) = 0,$	$z \in \Omega$	known.
$J_{\delta\eta}u(z,t) = 0,$	$(z,t) \in \partial\Omega \times (0,T]$	known.
$J_{\delta\eta}f(z)$	$z \in \Omega$	known.
$J_{\delta\eta}u(z,t),$	$(z,t) \in \Omega \times (0,T)$	unknown.

Then, the numerical method will find an approximation $J_\delta P^\epsilon$ which is expected to converge to p as ϵ, δ and the step size tend to zero. That is what it is shown in the results bellow. The general estimate is

$$\|p - J_\delta P^\epsilon\|_2 \leq \|p - J_\delta p\|_2 + \|J_\delta p - J_\delta P^\epsilon\|_2 \tag{4-51}$$

$$\leq C_1\Delta t + \|J_\delta p - J_\delta P^\epsilon\|_2. \tag{4-52}$$

The proof goes as follows: We define ω as follow

$$\sum_{i=1}^{m} a_{m-i+1}p(t_i) = h(t_m) - \omega(\Delta t, t_m), \tag{4-53}$$

where

$$\omega(\Delta t, t_m) = \int_0^{t_m} K(t_m - s)p(s)ds - \sum_{i=1}^{m} a_{m-i+1}p(t_i), \tag{4-54}$$

and

$$h(t_m) = \sum_{i=1}^{m} a_{m-i+1}P_i. \tag{4-55}$$

Then

$$\omega(\Delta t, t_m) = \sum_{i=1}^{m} a_{m-i+1}\left[P_i - p(t_i)\right] = \sum_{i=1}^{m} a_{m-i+1}\epsilon_i, \tag{4-56}$$

with

$$\epsilon_i = [P_i - p(t_i)] \tag{4-57}$$

Now

$$\omega(\Delta t, t_m) - \omega(\Delta t, t_{m-1}) = \sum_{i=1}^{m} a_{m-i+1}\epsilon_i - \sum_{i=1}^{m-1} a_{m-i}\epsilon_i \tag{4-58}$$

$$= a_1\epsilon_m + \sum_{i=1}^{m-1}\left[a_{m-i+1} - a_{m-i}\right]\epsilon_i. \tag{4-59}$$

From that we got

$$a_1\epsilon_m \quad = \quad [\omega(\Delta t, t_m) - \omega(\Delta t, t_{m-1})] - \sum_{i=1}^{m-1} [a_{m-i+1} - a_{m-i}]\,\epsilon_i. \tag{4-60}$$

Our task will be to bound the quantities in the right hand side, in order to apply Theorem 7.1 of [26].

Theorem 4.3.1. *Let the sequence $\zeta_0, \zeta_1, \ldots$ satisfy*

$$|\zeta_n| \leq A \sum_{i=0}^{n-1} |\zeta_i| + B_n, \qquad n = r, r+1, \ldots \tag{4-61}$$

where

$$A > 0, \qquad |B_n| \leq B, \qquad \sum_{i=0}^{r-1} |\zeta_i| \leq \eta. \tag{4-62}$$

Then

$$|\zeta_n| \leq (1+A)^{n-r}(B + A\eta), \qquad \eta = r, r+1, \ldots. \tag{4-63}$$

It is necessary to find bounds for the terms:

$$\max\nolimits_{1\leq m\leq M} |a_{m+1} - a_m|\,, \tag{4-64}$$

$$\max\nolimits_{1\leq m\leq M} |\omega(\Delta t, t_m) - \omega(\Delta t, t_{m-1})| \tag{4-65}$$

and for the initial errors

$$\sum_{i=0}^{r-1} |P_i - p(t_i)|.$$

Taking the first expression if $m \neq 1$

$$\begin{aligned} |a_{m+1} - a_m| \quad &= \quad \left| \int_0^{t_1} K(t_{m+1} - \tau) d\tau - \int_0^{t_1} K(t_m - \tau)) d\tau \right| \\ &\leq \quad \int_0^{t_1} |K(t_{m+1} - \tau) - K(t_m - \tau))|\, d\tau \\ &\leq \quad C_1 \Delta t \int_0^{t_1} d\tau = C_1 (\Delta t)^2. \end{aligned}$$

If $m = 1$

$$\begin{aligned}
|a_2 - a_1| &= \left| \int_0^{t_1} K(t_2-\tau)d\tau - \int_0^{t_1} K(t_1-\tau))d\tau \right| \\
&\leq \left| \int_0^{t_1} K(t_2-\tau)d\tau \right| + \left| \int_0^{t_1} K(t_1-\tau))d\tau \right| \\
&= \int_0^{t_1} K(t_1-\tau)d\tau + \int_{t_1}^{t_2} K(t_2-\upsilon))d\upsilon \\
&= \int_0^{t_2} K(t_1-\tau)d\tau \\
&= \sum_{n=1}^{\infty} f_n (2\Delta t)^{\alpha} E_{\alpha,\alpha+1}\left(-\lambda_n \left(2\Delta t\right)^{\alpha}\right).
\end{aligned}$$

Since that we get that

$$\max_{1\leq m\leq M} |a_{m+1} - a_m| = \sum_{n=1}^{\infty} f_n (2\Delta t)^{\alpha} E_{\alpha,\alpha+1}\left(-\lambda_n \left(2\Delta t\right)^{\alpha}\right) \chi_n(z_0) = (2\Delta t)^{\alpha} C_1.$$

Then, following the notation of the theorem above

$$0 < \frac{(2\Delta t)^{\alpha} \sum_{n=1}^{\infty} f_n E_{\alpha,\alpha+1}\left(-\lambda_n \left(2\Delta t\right)^{\alpha}\right) \chi_n(z_0)}{(\Delta t)^{\alpha} \sum_{n=1}^{\infty} f_n E_{\alpha,\alpha+1}\left(-\lambda_n \left(\Delta t\right)^{\alpha}\right) \chi_n(z_0)} \leq 2^{\alpha} C_1 = A.$$

The second expression gives:

$$\begin{aligned}
|\omega(\Delta t, t_m) - \omega(\Delta t, t_{m-1})| &= \left| \int_0^{t_m} K(t_m - s)p(s)ds - \sum_{i=1}^{m} a_{m-i+1} p(t_i) \right. \\
&\quad \left. - \int_0^{t_{m-1}} K(t_{m-1} - s)p(s)ds + \sum_{i=1}^{m-1} a_{m-i} p(t_i) \right| \\
&= \left| \int_0^{t_m} K(t_m - s)p(s)ds - \sum_{i=1}^{m} \int_{t_{i-1}}^{t_i} K(t_m - s)ds p(t_i) \right. \\
&\quad \left. - \int_0^{t_{m-1}} K(t_{m-1} - s)p(s)ds + \sum_{i=1}^{m-1} \int_{t_{i-1}}^{t_i} K(t_{m-1} - s)ds p(t_i) \right|
\end{aligned}$$

$$
\begin{aligned}
&= \Bigg|\sum_{i=1}^{m}\int_{t_{i-1}}^{t_i} K(t_m-s)\,[p(s)-p(t_i)]\,ds \\
&\quad -\sum_{i=1}^{m-1}\int_{t_{i-1}}^{t_i} K(t_{m-1}-s)\,[p(s)-p(t_i)]\,ds\Bigg| \\
&= \Bigg|\sum_{i=1}^{m}\int_{t_{i-1}}^{t_i} K(t_m-s)\,[p(s)-p(t_i)]\,ds \\
&\quad -\sum_{i=1}^{m-1}\int_{t_i}^{t_{i+1}} K(t_{m-1}-(r-\Delta t))\,[p(r-\Delta t)-p(t_i)]\,dr\Bigg| \\
&= \Bigg|\sum_{i=1}^{m}\int_{t_{i-1}}^{t_i} K(t_m-s)\,[p(s)-p(t_i)]\,ds \\
&\quad -\sum_{i=1}^{m-1}\int_{t_i}^{t_{i+1}} K(t_m-r)\,[p(r-\Delta t)-p(t_i)]\,dr\Bigg| \\
&= \Bigg|\int_0^{t_1} K(t_m-s)\,[p(s)-p(t_1)]\,ds \\
&\quad +\sum_{i=2}^{m}\int_{t_{i-1}}^{t_i} K(t_m-r)\,[p(r)-p(t_i)-p(r-\Delta t)+p(t_{i-1})]\,dr\Bigg| \\
&\le \int_0^{t_1} K(t_m-s)\,|p(s)-p(t_1)|\,ds \\
&\quad +\sum_{i=2}^{m}\int_{t_{i-1}}^{t_i} K(t_m-r)\,|p(s)-p(t_i)-p(r-\Delta t)+p(t_{i-1})|\,dr \\
&\le L\Delta t\int_0^{t_1} K(t_m-s)ds+2L\Delta t\sum_{i=2}^{m}\int_{t_{i-1}}^{t_i} K(t_m-r)dr \\
&\le 2L\Delta t\int_0^{t_1} K(t_m-s)ds+2L\Delta t\sum_{i=2}^{m}\int_{t_{i-1}}^{t_i} K(t_m-r)dr.
\end{aligned}
$$

Since that, then

$$
\begin{aligned}
\frac{1}{a_1}\left|\omega(\Delta t,t_m)-\omega(\Delta t,t_{m-1})\right| &\le 2L\Delta t\frac{1}{a_1}\left(\int_0^{t_m} K(t_m-s)ds\right) \\
&= 2L\Delta t\frac{1}{a_1}\left(\sum_{n=1}^{\infty} f_n\Big((m\Delta t)^\alpha E_{\alpha,\alpha+1}\left(-\lambda_n\,(m\Delta t)^\alpha\right)\Big)\chi_n(z_0)\right) \\
&\le 2L\Delta t\frac{1}{a_1}\left(\sum_{n=1}^{\infty} f_n\Big((T)^\alpha E_{\alpha,\alpha+1}\left(-\lambda_n\,(T)^\alpha\right)\Big)\chi_n(z_0)\right) \\
&= 2LC_2(\Delta t)^{1-\alpha}.
\end{aligned}
$$

Theorem 4.3.2. *Let p a Lipschitz continuous function in the interval $[0,T]$ and P obtained form the numerical method described above, then for r fixed*

$$|P_r - p(t_r)| \leq LC_r\Delta t, \tag{4-66}$$

with L being the Lipschitz constant of p and C_r a constant depending only on r.

Proof. We start with the case $r = 1$:

$$\begin{aligned}
|P_1 - p(t_1)| &= \left|\frac{h(t_1)}{a_1} - p(t_1)\right| \\
&\leq \frac{1}{a_1}\left|\int_0^{t_1} p(\tau)K(t_1-\tau,z)d\tau - p(t_1)\right| \\
&\leq \frac{1}{a_1}\int_0^{t_1} |p(\tau)-p(t_1)|\, K(t_1-\tau,z)d\tau \\
&\leq \frac{1}{a_1}\int_0^{t_1} K(t_1-\tau,z)d\tau\Delta t \\
&= L\Delta t
\end{aligned}$$

and, if $m = 2$

$$\begin{aligned}
|P_2 - p(t_2)| &= \frac{1}{a_1}\,|h(t_2) - a_2P_1 - a_1p(t_2)| \\
&= \frac{1}{a_1}\left|\int_0^{t_2} p(\tau)K(t_2-\tau)d\tau - a_2P_1 - a_1p(t_2)\right| \\
&= \frac{1}{a_1}\left|\int_0^{t_1} [p(\tau)-P_1]\,K(t_2-\tau)d\tau + \int_0^{t_1} [p(\tau)-p(t_2)]\,K(t_2-\tau)d\tau\right| \\
&\leq \frac{1}{a_1}C\Delta t\left|\int_0^{t_1} K(t_2-\tau)d\tau\right| + \frac{1}{a_1}C\Delta t\left|\int_{t_1}^{t_2} K(t_2-\tau)d\tau\right| \\
&= \frac{1}{a_1}L\Delta t a_1 + \frac{1}{a_1}L\Delta t a_2 \\
&= L\Delta t\frac{(2\Delta t)^\alpha}{a_1}\sum_{n=1}^{\infty} f_n\left(E_{\alpha,\alpha+1}\left(-\lambda_n\,(2\Delta t)^\alpha\right)\right)\chi_n(z_0) \\
&\leq LC_r\Delta t
\end{aligned}$$

Supposing the affirmation is true for $r-1$, then

$$
\begin{aligned}
|P_r - p(t_r)| &= \left| \frac{h(t_r)}{a_1} - \sum_{i=1}^{r-1} \frac{a_{r-i+1}P_i}{a_1} - p(t_r) \right| \\
&= \left| \int_0^{t_r} \frac{p(\tau)K(t_r-\tau)d\tau}{a_1} - \sum_{i=1}^{r-1} \frac{a_{r-i+1}P_i}{a_1} - p(t_r) \right| \\
&= \left| \sum_{i=1}^{r-1} \int_0^{t_r} \frac{p(\tau)K(t_r-\tau)d\tau}{a_1} - \sum_{i=1}^{r-1} \frac{a_{r-i+1}P_i}{a_1} - p(t_r) \right| \\
&= \frac{1}{a_1} \left| \sum_{i=1}^{r} \int_{t_{i-1}}^{t_i} p(\tau)K(t_r-\tau)d\tau - \sum_{i=1}^{r-1} a_{r-i+1}P_i - a_1 p(t_r) \right| \\
&= \frac{1}{a_1} \left| \sum_{i=1}^{r} \int_{t_{i-1}}^{t_i} p(\tau)K(t_r-\tau)d\tau \right. \\
&\quad \left. - \sum_{i=1}^{r-1} \int_{t_{i-1}}^{t_i} K(t_r-\tau,z)d\tau P_i - \int_{t_{r-1}}^{t_r} K(t_r-\tau,z)d\tau p(t_m) \right| \\
&= \frac{1}{a_1} \left| \sum_{i=1}^{r-1} \int_{t_{i-1}}^{t_i} [p(\tau)-P_i]K(t_r-\tau)d\tau \right. \\
&\quad \left. + \int_{t_{r-1}}^{t_r} [p(\tau)-p(t_r)]K(t_r-\tau)d\tau \right| \\
&\leq \frac{1}{a_1} \left| \sum_{i=1}^{r-1} \int_{t_{i-1}}^{t_i} [p(\tau)-P_i]K(t_r-\tau)d\tau \right| \\
&\quad + \frac{1}{a_1} \left| \int_{t_{r-1}}^{t_r} [p(\tau)-p(t_r)]K(t_r-\tau)d\tau \right| \\
&\leq \frac{L\Delta t}{a_1} \sum_{i=1}^{r-1} \int_{t_{i-1}}^{t_i} K(t_r-\tau)d\tau + \frac{L\Delta t}{a_1} \int_{t_{r-1}}^{t_r} K(t_r-\tau,z)d\tau \\
&= \frac{L\Delta t}{a_1} \sum_{i=2}^{r} a_i + \frac{L\Delta t}{a_1} a_1 \\
&= \frac{L\Delta t}{a_1} \sum_{n=1}^{\infty} f_n (r\Delta t)^\alpha E_{\alpha,\alpha+1}\left(-\lambda_n (r\Delta t)^\alpha\right) \chi(z_0) \\
&\leq LC_r \Delta t
\end{aligned}
$$

□

Returning to 4-60, and applying the result we just get, we obtain

$$\begin{aligned} |\epsilon_m| &= \frac{1}{|a_1|}\left|[\omega(\Delta t, t_m) - \omega(\Delta t, t_{m-1})] - \sum_{i=1}^{m-1}[a_{m-i+1} - a_{m-i}]\,\epsilon_i\right| \\ &\leq \frac{1}{|a_1|}|\omega(\Delta t, t_m) - \omega(\Delta t, t_{m-1})| + \frac{1}{|a_1|}\sum_{i=1}^{m-1}|a_{m-i+1} - a_{m-i}|\,|\epsilon_i| \\ &\leq 2LC_2(\Delta t)^{1-\alpha} + A\sum_{i=1}^{m-1}|\epsilon_i|. \end{aligned}$$

Calling $B = LC_2(\Delta t)^{1-\alpha}$ and $\eta = LC_m\Delta t$, that let us conclude from theorem (4.3.1)

$$|\epsilon_m| \;\leq\; (1+A)^{n-r}(LC_2(\Delta t)^{1-\alpha} + ALC_r\Delta t) \xrightarrow{\Delta t \longrightarrow 0} 0$$

4.3.3. Results

Our strategy is to implement the finite difference method of [32] and the estimation of $p(t)$ by the method explained above. Numerical results are shown for the following time-fractional diffusion problem:

$$\left.\begin{array}{llll} D_t^\alpha u(z,t) - (Lu)(z,t) & = p(t)f(z), & z \in \Omega & t \in (0,T) \\ u(z,t) & = 0, & z \in \partial\Omega & t \in (0,T) \\ u(z,0) & = 0, & z \in \bar{\Omega} & t \in (0,T) \end{array}\right\} \tag{4-67}$$

where,

$$Lu(x,y) = \frac{\partial}{\partial x}\left(a_{11}(x,y)\frac{\partial}{\partial x}u(x,y)\right) + \frac{\partial}{\partial y}\left(a_{22}(x,y)\frac{\partial}{\partial y}u(x,y)\right). \tag{4-68}$$

Example 1

For the diffusion operator, let $a_{11}(x,y) = 1$ and $a_{22}(x,y) = 1$. Moreover, let $f = 100sin(\pi x)sin(\pi y)$ and $p = sin(5\pi t)$. Table **4-6** shows results for noisy data without mollification ($\eta = 0$) and results with mollification with many η values, both with grid size in space $h = 1/32$ and in time $k = 1/64$.
Figure **4-2** illustrates the difference in the identification.

Example 2

Let $a_{11}(x,y) = 1$, $a_{22}(x,y) = 1$, $f = 100sin(\pi x)sin(\pi y)$ and $p(t) = t^2$. Again, we compare results with and without mollification.
Figure **4-3** illustrates the results for this example.

Table 4-6.: Error norms with mollification, $\epsilon = 0.1$ and different values of η and α.

$\alpha \backslash \eta$	0	1	2	3	4
0,1	0,01545	0,013749	0,011137	0,011152	0,011152
0,5	0,072285	0,063794	0,064744	0,064723	0,064723
0,7	0,09096	0,082511	0,083209	0,083188	0,083188
0,9	0,073896	0,068144	0,06647	0,066468	0,066468

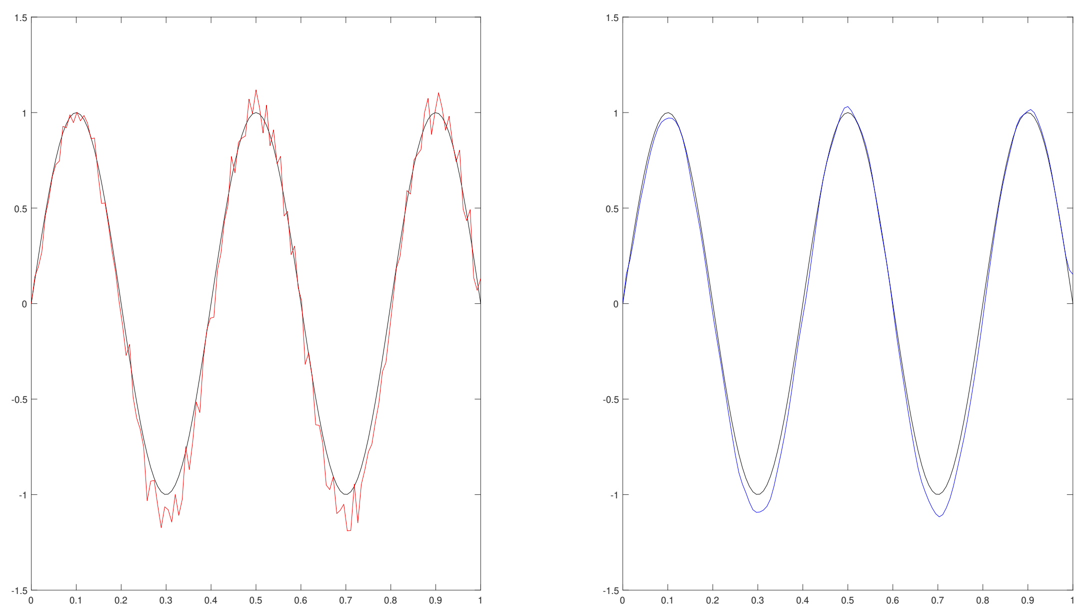

Figure 4-2.: Comparison between the approximation with and without mollification and the exact solution for $h = 1/16$, $k = 1/128$ and $\alpha = 0.9$

Table 4-7.: Error norms without mollification $\epsilon = 0.1$ and different values of α.

$\alpha \backslash \eta$	0	1	2	3	4
0,1	0,01218	0,0079	0,00657	0,00615	0,00598
0,5	0,01603	0,01043	0,00942	0,00908	0,00914
0,7	0,01973	0,01174	0,01034	0,00943	0,00923
0,9	0,03686	0,01219	0,01366	0,01041	0,00921

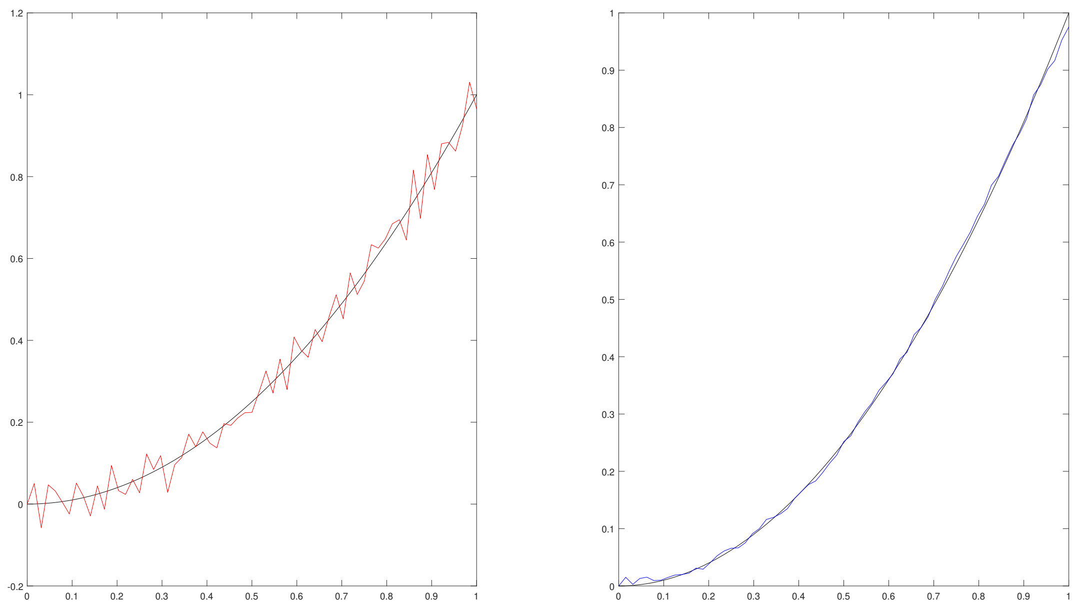

Figure 4-3.: Comparison between the approximation with and without mollification and the exact solution for $h = 1/16$, $k = 1/64$ and $\alpha = 0.9$

Example 3

Let $a_{11}(x, y) = 1$, $a_{22}(x, y) = 1$, $f = 100 sin(\pi x)sin(\pi y)$ and

$$p(t) = \begin{cases} t - 0.2, & t \in [0.2, 0.5] \\ 0.8 - t, & t \in [0.5, 0.8] \\ 0 & \text{otherwise.} \end{cases}$$

Again, we compare results with and without mollification in the table **4-8**.

Table 4-8.: Error norms with mollification, $\epsilon = 0.1$ and different values of η and α.

$\alpha \backslash \eta$	0	1	2	3	4
0,1	0,013321	0,009897	0,009312	0,009185	0,009206
0,5	0,029103	0,025445	0,024606	0,02444	0,0244
0,7	0,037986	0,031672	0,030359	0,029933	0,029842
0,9	0,062472	0,027119	0,021259	0,018064	0,017686

Figure **4-4** illustrates the results for this example.

As conclusions of our work in this chapter an in particular in this section, we mention the following:

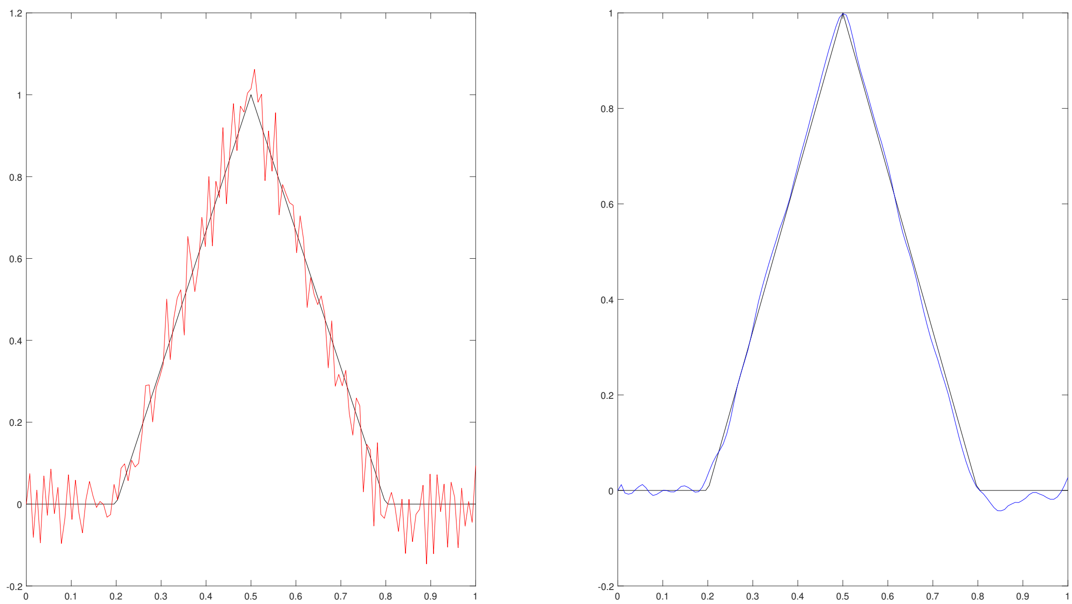

Figure 4-4.: Left: Identification without mollification. Right: Identification with mollification, $h = 1/16$, $k = 1/128$ and $\alpha = 0.9$

1. The combination of finite difference methods and discrete mollification is a successful procedure for the identification of forcing term factors in time fractional diffusion equations.

2. If the factor is the space dependent factor, that is, the discharge intensity, the overposed data is a complete distribution of the concentration at the final time.

3. If the factor is the time dependent factor, that is, the attenuation coefficient, the overposed data is a complete history at an interior point.

4. We are confident that other forcing term identification problems are solvable by the same strategy of finite difference and mollification. Actually we expect to work in other problems of this kind in the near future.

5. Efficient parameter estimation in a solute transport model

Our goal is the numerical identification of solute transport parameters in a one dimensional space fractional advection dispersion equation for the concentration of the solute. The unknown parameters are the fractional derivative order, the dispersion coefficient and the average velocity. The direct problem is solved by a backward Euler method in which the dispersion term consisting on a Caputo fractional derivative, is discretized by the classical L2 finite difference method. The parameter estimation is implemented through a history matching procedure enhanced by discrete mollification. We consider two different inverse problems, characterized by two types of overposed data: The complete time distribution of the concentration at a fixed interior location and the complete space distribution of the concentration at the final time of the experiment. The ability of the proposed parameter estimation procedure is verified by illustrative numerical examples.

5.1. Introduction

Contaminant transport in porous media and in rivers is one of the main topics of study in hydrodynamic dispersion theory ([11, 48, 8]). The dispersion is of two types: Fickian, i.e., based on Fick's law and non-Fickian or anomalous. The Fickian dispersion is associated with advection dispersion equations (ADE) which include classical derivatives only and the anomalous dispersion is modeled by fractional advection dispersion equations (FADE) which include fractional derivatives and may include classical derivatives as well.

The time fractional differential operators are operators with memory and the space fractional differential operators are nonlocal operators. Many models of science and engineering require the combination of time and space fractional differential operators. A recent survey of real world applications of fractional calculus is [45].

Many interesting and challenging inverse problems consist on estimating unknown parameters in differential equations and there are different ways to solve them, many of which are iterative in nature and require the solution of the associated direct problem in each iteration. Some of these problems arise in the study of solute transport in soils or aquifers whose regime is quite frequently of anomalous diffusion and the equations are space fractional dispersion equations (sFADE).

Based on time fractional differential equations (tFADE), there are ill-posed problems, namely, the problems investigated in [31, 50] and there are well-posed problems, for instance [13]. Based on sFADE's there are parameter estimation problems that are well-posed, namely [7, 23] and there are other estimation problems that are numerically solved by a history matching method combined with Tikhonov regularization. Among them, we mention [48] and [52].

In [48] the authors consider a parameter estimation problem based on a one dimensional sFADE defined on the interval $[0, L]$. The necessary overposed data is an interior point concentration measurements for all time. They consider a Riemann-Liouville fractional derivative, a history matching process based on a gradient iterative method of minimization combined with Tikhonov regularization and boundary condition of Dirichlet type at $x = 0$ and Neumann homogeneous at $x = L$. In [52] the authors solve a similar problem by a history matching algorithm combined with Tikhonov regularization. The differences are: The overposed data is a final concentration known for all $x \in [0, L]$ and the boundary conditions are Dirichlet homogeneous at both endpoints. Both papers implement Tikhonov regularization without any proof of ill-conditioning.

Both authors include regularization without any proof of ill-posedness. Given an anomalous transport equation consisting on a one dimensional space fractional advection dispersion equation (sFADE), our goal is to solve several parameter identification problems by a history matching procedure. The main features of our work are:

1. The fractional derivatives are Caputo fractional derivatives of order $\alpha \in (1, 2)$.

2. Our equations admit different types of initial and boundary conditions.

3. We have no proof of ill-posedness and suspect that, if it is ill-posed, it is only mildly ill-posed.

4. Our method allows for the optional implementation of discrete mollification as in [2, 3]. The effect of this addition is stabilization and/or acceleration of computations.

5. Our history matching approaches are based on the Nelder Mead Simplex Method and, unlike [48] and [52], the numerical method of solution of the direct problem is an implicit backward Euler method together with the known L2 finite difference formula for the Caputo fractional derivative ([30, 37, 43]).

On the one dimensional approach, common to the three works, it is appropriate to cite [11]: *A typical question that a contaminant hydrogeologist wishes to answer is: How far and how fast will a tracer move? As a first approximation, this reduces most problems to one spatial dimension.* Moreover, in [8] one dimensional FADE show very well performance in comparison with more complex methods for particle transport in rivers.

The rest of the chapter is organized as follows: The next section introduces the direct problem and section 3 deals with the numerical solution of the direct problem and both parameter estimation problems based on history matching procedures. The numerical experiments appear in section 4 and the section ends with some final remarks and conclusions.

5.2. Direct problem

We are interested in the following one dimensional FADE for the tracing of a non reactive contaminant:

$$\frac{\partial C}{\partial t} = -v\frac{\partial C}{\partial x} + D\frac{\partial^\alpha C}{\partial x^\alpha} + f(x,t) \tag{5-1}$$

where C is the solute concentration, v is the pore-water velocity, D is the dispersion coefficient, $0 < t$, $x \in [0, L]$, $\frac{\partial^\alpha C}{\partial x^\alpha}$ is the Caputo fractional derivative of the concentration C of order α with $1 < \alpha \leq 2$ and $f(x,t)$ is a forcing term.
Together with equation (5-1) there are an initial condition and a set of boundary conditions. Examples of them are (see [48]):

$$C(x,0) = 0 \quad \text{initial condition} \tag{5-2}$$

$$C(0,t) = C_0 \text{ left boundary condition, Dirichlet type} \tag{5-3}$$

$$\frac{\partial C}{\partial x}|_{x=L} = 0 \quad \text{right boundary condition, Neumann type} \tag{5-4}$$

The direct problem consists on finding C that satisfies (5-1)-(5-4) assuming all parameters are known. Our method of solution for all direct problems based on equation (5-1) is the L2 method. Other initial and boundary conditions will be consider in the numerical experiments.

5.3. The inverse problems

If any of the parameters present in equations (5-1)-(5-4) is unknown, an additional set of measurements is required in order to identify the missing parameters. In this chapter we consider two types of overposed data:

1. Measurements of concentration at a fixed interior location for all time. That is, we assume an a priori knowledge of the concentration C at a particular observation point x_*, that we denote $C^{obs}(t)$ for all $t \geq 0$.

2. Measurements of concentration at the final time for all space locations. At the final time T the concentration $C_{obs}(x)$ is known for all $x \in [0, L]$.

Parameter estimation problems belong to the category of inverse problems. A given direct problem may be associated to several inverse problems, depending on the part of data information that is missing.
In order to solve our parameter identification problem we prepare the following setting:

1. A vector P consisting on the unknown parameters to be approximated, for instance, if v and α are the sought parameters, $P = [v, \alpha]$.

2. A finite difference method of solution of the direct problem (5-1)-(5-4).

3. An optional acceleration method, which in our case is the discrete mollification method.

4. A history matching procedure.

We show details for the first type of overposed data. The second case is similar.

5.3.1. Numerical solution of the direct problem

The selected method is a backward Euler finite difference method. Let $\{0 = x_0, x_1, x_2, \ldots, x_M = L\}$ be a space grid with uniform discretization parameter $h = L/M$ and k a time discretization parameter so that the time grid is $t_n = nk, n = 0, 1, \ldots$ Moreover, let $T = Nk$ be the last time of the experiment, that is, $n = 0, 1, \ldots, N$.
By C_j^n we denote the aproximation of $C(x_j, t_n)$ and, without loss of generality, we suppose the observation point x_* is x_J for some $J \in \{1, 2, \ldots, M-1\}$.
Finally, we denote $f_i^n = f(x_i, t_n)$. Furthermore, for space dependent velocity v and dispersion coefficient D we denote $v_j = v(x_j)$ and $D_j = D(x_j), j = 0, 1, \ldots, M$.
The discretized version of equation (5-1) consists on a combination of the backward Euler method and the L2 finite difference formula for the fractional derivative ([30, 37, 43]). It is

$$\frac{C_i^{n+1} - C_i^n}{k} = -v_i \frac{C_i^{n+1} - C_{i-1}^{n+1}}{h} + D_i I + f_i^{n+1} \tag{5-5}$$

where I is the approximation of the evaluation at grid points of the Caputo fractional derivative $\frac{\partial^\alpha C}{\partial x^\alpha}(x_{j+1}, t_{n+1})$, which is given by

$$\frac{1}{h^\alpha \Gamma(3-\alpha)} \sum_{j=0}^{i-1} b_j \left[C_j^{n+1} - 2C_{j+1}^{n+1} + C_{j+2}^{n+1}\right] \tag{5-6}$$

where $b_j = (i-j)^{2-\alpha} - (i-j-1)^{2-\alpha}$.

5.3.2. History matching

We consider the case in which the overposed data is given by a time distribution of concentration at a fixed interior location. Let $P = [v, \alpha]$ be the vector of unknown parameters. This is an example, all other combinations of parameters are possible. Thus, in (5-1)-(5-4) the parameters v and α are unknown. The inverse problem consists on identifying P based on the set of equations (5-1)-(5-4) and the additional measurements of the concentration at the observation point x_J, i.e. $C^{obs}(t_n)$ for $n = 1, 2, \ldots$

The history matching is based on the minimization of a cost functional. In our case it is

$$J(P) = \left(\frac{1}{N} \sum_{n=1}^{N} \left[C_J^n - C^{obs}(t_n) \right]^2 \right)^{1/2}$$

where each numerical solution C_J^n is obtained from the sFADE with parameters taken from the parameter vector P.
The subtle point is the introduction of the discrete mollification operator. For that matter we follow [1] and apply mollification in the dispersion term, which in our case, is the fractional derivative term. Estimate (2-21) of the previous theorem is crucial here.
For the case of overposed data given by a concentration for all locations at the final time, the algorithm is analogous. In this case the additional measurements of the concentration at the final time T are $C_{obs}(x)$ for $x \in [0, L]$. In this case the cost functional is

$$J(P) = \left(\frac{1}{M} \sum_{j=1}^{M} \left[C_j^N - C_{obs}(x_j) \right]^2 \right)^{1/2}$$

where each numerical solution C_J^n is obtained from the sFADE with parameters taken from the parameter vector P.
In the first case, the history matching algorithm with mollification is:

Algorithm: History Matching with mollification

Overposed data is given by a time distribution of concentration at a fixed interior location

1. Choose initial P, a maximum number of iterations $maxiter$ and a tolerance ε.
2. Set $iter = 0$
3. While $iter < maxiter$
   a) Choose a positive integer η as support parameter of mollification and prepare the mollified direct problem corresponding to (5-5)-(5-6) given by

   $$\frac{C_i^{n+1} - C_i^n}{k} = -v_i \frac{C_i^{n+1} - C_{i-1}^{n+1}}{h} + D_i I_\eta + f_i^{n+1} \tag{5-7}$$

   where I_η is the mollified approximation of the evaluation at grid points of the Caputo fractional derivative, that is, $\frac{\partial^\alpha C}{\partial x^\alpha}(x_{j+1}, t_{n+1})$, which is given by

   $$\frac{1}{h^\alpha \Gamma(3-\alpha)} \sum_{j=0}^{i-1} 2C_\eta b_j \left[[J_\eta C^{n+1}]_{j+1} - C_{j+1}^{n+1} \right] \tag{5-8}$$

   where $b_j = (i-j)^{2-\alpha} - (i-j-1)^{2-\alpha}$.

   b) Solve the mollified direct problem corresponding to parameter vector P

c) Find $P_m = \arg\min_P J(P)$

d) Set $P = P_m$

e) If $J(P) < \varepsilon$
Print $P, iter, C_J^n$
Stop

f) Set $iter = iter + 1$
end While

4. Print $P, iter, C_J^n$ and a failure message since a normal exit was not achieved.

The numerical implementation of the optimization procedure of step 3. (c) is based on a restarted version of the Nelder-Mead Simplex Method (MATLAB `fminsearch` function.) See [25] for details on the method. The **history matching algorithm without mollification**

is the same, except that steps 3. (a) and (b) are the following:

- 3 (a) State the numerical method for the direct problem given by equations (5-5)-(5-6).
- 3 (b) Solve the direct problem corresponding to parameter vector P.

The history matching algorithm in the case of overposed data given by a final concentration at all locations, is analogous and we omit the details.

5.4. Numerical experiments

Example 5.4.1. This example is took from [39]. It confirms the validity of the schemes solving the direct problem:

$$\begin{cases} u_t(x,t) &= c(x)u_x^\alpha(x,t) + q(x,t), & x \in (0,1), t > 0; \\ u(x,0) &= x^2 - x^3, & x \in [0,1]; \\ u(0,t) &= u(1,t) = 0, & t > 0; \\ c(x) &= \Gamma(1.2)x^{1.8}, & x \in [0,1]; \\ q(x,t) &= (6x^3 - 3x^2)e^{-t}, & x \in [0,1], t > 0. \end{cases}$$

The solution of this initial-boundary problem is $u(x,t) = (x^2 - x^3)e^{-t}$. With both schemes the solution is approximated satisfactorily. The errors corresponding to the mollified scheme with $\eta = 2$ and the L_2 scheme are shown in Table **5-1**.

Example 5.4.2. Now we have homogeneous Dirichlet boundary conditions, initial data given by $u(x,0) = x^2 - x^3$ and source term $q(x,t) = (6x^3 - 3x^2)e^{-t}$. Tables **5-2** and **5-3** show results of the identification based on overposed data given by a complete history at the

Table 5-1.: Solution of direct problem by Mollified scheme and scheme L2

h=k	Mollified	L_2
1/8	0.00671	0.00564
1/16	0.00498	0.0035
1/32	0.00314	0.00204
1/64	0.0018	0.00114
1/128	0.00098	0.00062

Table 5-2.: Error for different values of η, $\alpha = 1.7$ and $h = k = 1/100$.

η	v	D	fval	iter
0	0,500012535	1,500000987	3,77007E-08	74
2	0,499989387	1,500001585	2,7726E-08	73
5	0,499978474	1,500000692	1,91952E-08	72
8	0,499963412	1,500001648	3,54588E-08	67

Table 5-3.: Error for different values of α, $\eta = 2$ and $h = k = 1/100$.

α	v	D	fval	iter
1,1	0,499917954	1,499947596	1,24976E-06	60
1,5	0,499977265	1,499996713	5,32297E-08	75
1,7	0,499989387	1,500001585	2,7726E-08	73
1,9	0,500008618	1,500001769	4,56247E-08	62

interior point $x = 0.5$.
Here we show the error of the approximation using different values of α, taking $\eta = 2$ and $(v_0, D_0) = (0, 1)$ as the initial estimate.

Example 5.4.3. This example deals with overposed data given by a complete distribution at the final time. Boundary conditions are a combination Dirichlet-Neumann given by

$$u(0,t) = exp(-t), \quad \frac{\partial u}{\partial x}|_{x=1} = 0,$$

initial condition is $u(x, 0) = (x-1)^2$ and the source term is

$$q(x,t) = -\frac{e^{-t}}{\Gamma(3-\alpha)}\left[(x-1)^2 - 2v(x-1) + 2D(x^{2-\alpha})\right]$$

Table 5-4 shows results for the simultaneous identification of $v = 1, D = 0.5$ and several values of the order of differentiation α. No mollification is implemented and this is one of the reasons we believe that if the problem is ill-posed, it is not very ill-posed. This is a subject of further work.

Table 5-4.: Error for different values of α and $h = k = 1/100$.

α	α_{approx}	v	D	fval	iter
1,1	1,099981081	1,00004874	0,50004461	1,7816E-08	154
1,5	1,499944085	1,0000253	0,50002746	3,0331E-09	126
1,7	1,699955028	1,00002411	0,50002512	8,0513E-10	230
1,9	1,883730123	1,01416191	0,51159031	1,4001E-07	351

Final remarks and conclusions

1. Anomalous dispersion of solutes in soil is the subject of current research in several fields, including numerical analysis.

2. It is possible to estimate parameters for one dimensional solute transport models based on space fractional advection dispersion equations.

3. The overposed data can be of two types: An interior location distribution of concentration at all times and the final time concentration for all space locations.

4. It is worth considering extensions of our method to other solute transport situations, for instance, 2D and 3D models.

6. Conclusions and final remarks

Interactions between inverse problems and fractional derivatives are a huge research field in which new results appear daily. In this thesis we could establish original, stable and efficient methods to solve several inverse problems of interest in the vast area of flow in porous media and anomalous diffusion. All the equations correspond to solute transport in porous media, thus the dependent variable is solute concentration.
The main achievements in this thesis are:

1. For a two dimensional time fractional diffusion equation with a separable forcing term $f(z)p(t)$, we solved the inverse problem consisting on the estimation of the discharge magnitude $f(z)$. As overposed data a noisy version of the concentration distribution at the final time is available. The regularization is achieved by discrete mollification. Our results are published in [16].

2. For the same two dimensional time fractional diffusion equation with a separable forcing term $f(z)p(t)$, we solved an identification problem consisting on the estimation of the attenuation coefficient $p(t)$. The overposed data is a noisy solute concentration distribution at the final time. Discrete mollification is the chosen regularization tool.

3. Parameter estimation problems in the framework of one dimensional space fractional advection-dispersion equations are included in this thesis. There are simultaneous identification of parameters for equations with different boundary conditions. The selected procedure to solve the inverse problems is history matching coupled with optimization by the Nelder-Mead Simplex method.

4. All MATLAB routines are original, except some mollification routines prepared by C.D. Acosta. Our routines are part of the results obtained in this thesis.

There are other original ideas throughout the thesis, some of which constitute work in progress. Some of these ideas come from fruitful conversations with professor Pep Mulet of University of Valencia, Spain, who invited me for a six month visit. Comparison with other regularization strategies as Tikhonov method, is an interesting approach to study subsequently.
The MATLAB routines and three papers, two of which are work in progress, can be found in
https://medellin.unal.edu.co/~cemejia/

Our current research work consists on the completion of the preprints related to the topics of chapters 4 and 5 of the thesis and the addition of Tikhonov method as a second regularization strategy. What about the not so immediate future? Fractional differential equations and inverse problems constitute a successful pair. We expect they will stay together for many years. It was very satisfying to work with this couple and we expect to keep working on this subject for many more years.

A. The Mollification in Higher Dimensions

A.1. General Case

Given $\delta > 0$, $p > 0$ in $\mathbb{R}$, we define

$$A_{\delta p} = \left(\int_{B_{p/\delta}} exp(-\|x\|^2)dx \right)^{-1} \tag{A-1}$$

where

$$B_r := \{x \in \mathbb{R}^n / \|x\| < r\} \tag{A-2}$$

Now, we take a truncated Gaussian kernel:

$$\kappa_{\delta p}(t) = \begin{cases} A_{\delta p}\delta^{-1}exp(-\|t\|^2/\delta^2), & \|t\| \leq p \\ 0, & \|t\| > p \end{cases} \tag{A-3}$$

This kernel satisfies

- $\kappa \geq 0$.
- $\kappa \in C^\infty(B_p)$.
- $\kappa \equiv 0$ outside $\bar{B}_p$.
- $\int_{\mathbb{R}^n} \kappa_{\delta p} = 1$

Definition A.1.1. *Set $f : \mathbb{R}^n \mapsto \mathbb{R}$ locally integrable, we define its δp-mollification, denoted $J_{\delta p} f$, as the convolution of f with $\kappa_{\delta p}$. That is,*

$$\begin{aligned} J_{\delta p} f(t) &= (\kappa_{\delta p} * f)(t) && \text{(A-4)} \\ &= \int_{\mathbb{R}^n} \kappa_{\delta p}(t-s) f(s) ds && \text{(A-5)} \\ &= \int_{B_p(t)} \kappa_{\delta p}(t-s) f(s) ds && \text{(A-6)} \\ &= \int_{B_p} \kappa_{\delta p}(-s) f(t+s) ds && \text{(A-7)} \end{aligned}$$

It will be taken $p = 3\delta$, then

$$A_{\delta p} = \left(\int_{B_{p/\delta}} exp(-\|x\|^2)dx\right)^{-1} = \left(\int_{B_3} exp(-\|x\|^2)dx\right)^{-1} \tag{A-8}$$

Definition A.1.2. *Set $X = \{x\alpha / X_\alpha = X_0 + \alpha h, \alpha \in \mathbb{Z}^n\}$ a rectangular grid in $\mathbb{R}^n$ with step size $h \in \mathbb{R}^+$. Set $G : X \mapsto \mathbb{R}$ a function defined for $G(X_\alpha) = y_\alpha$. Also, set*

$$S_\alpha(j) = (X_{\alpha_{j-1}} + X_{\alpha_j})/2 \tag{A-9}$$

$$I_\alpha = \prod_{j=1}^{n} [S_\alpha(j), S_\alpha(j+1)) \tag{A-10}$$

$$f(t) = \sum_{\alpha \in \mathbb{Z}^n} y_\alpha \chi_\alpha(t) \tag{A-11}$$

with χ_α the characteristic function of the n-cell I_α. Then for $\delta > 0$ and η a non negative integer, we define the $\delta\eta$-mollification of G as the δp- mollification of f with

$$p = (\eta + 1/2)h \tag{A-12}$$

that is,

$$J_{\delta\eta}G(x) = J_{\delta p}f(x) \tag{A-13}$$

We are interested on the value of $J_{\delta\eta}G$ in the discrete domain X. Let

$$t_\beta(j) = (\beta_j - 1/2)h, \ \beta \in \mathbb{Z}^n \tag{A-14}$$

$$P_\beta = \prod_{j=1}^{n} [t_\beta(j), t_\beta(j+1)) \tag{A-15}$$

We can write

$$J_{\delta\eta}G(X_\alpha) = J_{\delta\eta}f(X_\alpha) \tag{A-16}$$

$$= \int_{B_p} \kappa_{\delta p}(-s) f(X_\alpha + s)ds \tag{A-17}$$

$$= \sum_{|\beta| \leq \eta} \int_{P_\beta} \kappa_{\delta p}(-s) f(X_\alpha + s)ds \tag{A-18}$$

and it satisfies

$s \in P_\beta$ if and only if $X_\alpha + s \in I_{\alpha+\beta}$. Later

$$J_{\delta\eta}G(X_\alpha) = \sum_{|\beta| \leq \eta} w_\beta y_{\alpha+\beta}, \text{where } w_\beta = \int_{P_{beta}} \kappa_{\delta p}(-s)ds \tag{A-19}$$

that is, a discrete convolution of a vector of data y and some vector of weights w. The vector w satisfies

$$\sum_{i=-\eta}^{\eta} w_i = 1 \tag{A-20}$$

$$\sum_{i=-\eta}^{\eta} i w_i = 0 \tag{A-21}$$

Before formulate our principal theorem, it will reminded the Taylor's Theorem for multivariate functions.

Taylor's Theorem *If $f : \mathbb{R}^n \mapsto \mathbb{R}$ is C^{k+1} in the point $b \in \mathbb{R}^n$. Then there exist $h_b : \mathbb{R}^n \mapsto \mathbb{R}$ such that*

$$f(x) = \sum_{|\alpha \leq k|} \frac{D^\alpha f(b)}{\alpha!}(x-b)^\alpha + \sum_{|\alpha|=k} h_b(x)(x-b)^\alpha \tag{A-22}$$

and

$$\lim_{x \mapsto b} h_b(x) = 0 \tag{A-23}$$

Theorem A.1.3. *Set g a function defined on $\mathbb{R}^2$ with derivatives of order 4 continuous and bounded in $\mathbb{R}$. Let G the discrete version of g defined on X.*

- *Stability and Consistency: If G^ϵ is another discrete function defined on X, such that*

$$\|G^\epsilon - G\|_\infty \leq \epsilon \tag{A-24}$$

then for each compact set $K \subset \mathbb{R}^n$ there exists a constant C_K such that for all $x \in K$

$$\|J_{\delta\eta} G^\epsilon - J_{\delta\eta} G\|_\infty \leq \epsilon, \tag{A-25}$$

$$\|J_{\delta\eta} G^\epsilon - J_{\delta\eta} g\|_\infty \leq C_K h^2. \tag{A-26}$$

- *Mollified Numerical Differentiation: Moreover,*

$$\ldots \tag{A-27}$$

Proof. Stability:

$$|J_{\delta\eta} G^\epsilon(x) - J_{\delta\eta} G(x)| = \left| \sum_{|\beta| \leq \eta} w_\beta G^\epsilon(x) - G(x) \right| \tag{A-28}$$

$$\leq \sum_{|\beta| \leq \eta} w_\beta \left| G^\epsilon(x) - G(x) \right| \tag{A-29}$$

$$= |G^\epsilon(x) - G(x)| \sum_{|\beta| \leq \eta} w_\beta \leq \epsilon \tag{A-30}$$

Consistency: let $X_\alpha \in K$ then for Taylor's Theorem, for each $\beta \in \mathbb{Z}^n$, with $|\beta| \leq \eta$, there exists $\zeta_\beta \in \hat{K} = \{z \in K/d(z, \partial K) \geq p\}$ such that

$$g(X_{\alpha+\beta}) = g(X_\alpha) + h\beta \cdot \nabla g(X_\alpha) + \sum_{|\beta|=2} \frac{D^\beta g(\zeta_\beta)}{2}(h\beta)^\beta \tag{A-31}$$

Thus

$$\begin{aligned} J_{\delta\eta}G(X_\alpha) &= \sum_{|\beta|\leq\eta} w_\beta g(X_{\alpha+\beta}) && \text{(A-32)} \\ &= \sum_{|\beta|\leq\eta} w_\beta \left(g(X_\alpha) + h\beta \cdot \nabla g(X_\alpha) + \sum_{|\gamma|=2} \frac{D^\gamma g(\zeta_\beta)}{2}(h\beta)^\gamma \right) && \text{(A-33)} \\ &= g(X_\alpha) + \frac{h^2}{2} \sum_{|\beta|=2} \beta^\beta w_\beta D^\beta g(\zeta_\beta) && \text{(A-34)} \end{aligned}$$

□

B. Time Fractional Inverse Heat Conduction Problem

B.1. Direct Problem

Some discussion will be made about the direct problem, its outlining and theoretical considerations will be made here.

B.2. Inverse Problem

The Inverse Heat Conduction Problem is a classic one where a boundary is unknown and the determination of it, is the aim. Well, below a fractional version of this problem is presented and a approximation of its solution is obtained using the the Total Variation regularization. Our issue is given by

$$\begin{cases} {}_0D_t^{\alpha}u(x,y,t) - u_{xx}(x,y,t) - u_{yy}(x,y,t) = 0 & 0 < x < 1, y > 0, t > 0, \\ & 0 < \alpha \leq 1, \\ u(1,y,t) = g(x,y) & y \geq 0, t \geq 0 \\ u(x,y,0) = 0 & x > 0, y \geq 0 \\ u(x,0,t) = 0 & x > 0, t \geq 0 \\ u_y(x,y,0) = 0 & x > 0, y \geq 0 \\ u(x,y,t)|_{x\to\infty}, \quad \text{bounded} & x > 0, y \geq 0, \end{cases} \tag{B-1}$$

where the time derivative ${}_0D_t^{\alpha}u(x,y,t)$ is the Caputo fractional derivative of order $\alpha \in (0,1]$, defined by [38]

$${}_0D_t^{\alpha}u(x,y,t) = \frac{1}{\Gamma(1-\alpha)}\int_0^t \frac{\partial u(x,y,s)}{\partial s}\frac{ds}{(t-s)^{\alpha}}, \quad 0 < \alpha < 1 \quad , \tag{B-2}$$

$${}_0D_t^{\alpha}u(x,y,t) = \frac{\partial u(x,y,s)}{\partial s}, \qquad \alpha = 1. \tag{B-3}$$

We only have access to a noisy measurement g^{δ} which satisfies

$$\|g - g^{\delta}\|_{L^2} \leq \delta, \tag{B-4}$$

this problem is known to be ill-posed as it is proven in [50]. First of all we solve the problem below

$$\begin{cases} {}_0D_t^{\alpha}u(x,y,t) - u_{xx}(x,y,t) - u_{yy}(x,y,t) = 0 & 0 < x < 1, y > 0, t > 0, \\ & 0 < \alpha \leq 1, \\ u(0,y,t) = f(x,y) & y \geq 0, t \geq 0 \\ u(x,y,0) = 0 & x > 0, y \geq 0 \\ u(x,0,t) = 0 & x > 0, t \geq 0 \\ u_y(x,y,0) = 0 & x > 0, y \geq 0 \\ u(x,y,t)|_{x\to\infty}, \quad \text{bounded} & x > 0, y \geq 0, \end{cases} \tag{B-5}$$

applying the Fourier transform in this problem we get

$$\begin{cases} (i\eta)^{\alpha}\hat{u} - \hat{u}_{xx} + \zeta^2\hat{u} = 0 & 0 < x < 1, \\ \hat{u}(0,\zeta,\eta) = \hat{f}(\zeta,\eta), \\ \hat{u}(x,\zeta,\eta)|_{x\to\infty}, \quad \text{bounded} & x > 0. \end{cases} \tag{B-6}$$

The solution of this differential equation takes the form

$$\hat{u}(x,\zeta,\eta) = exp\left(-x\sqrt{(i\eta)^{\alpha} + \zeta^2}\right)\hat{f}(\zeta,\eta). \tag{B-7}$$

Thus the solution of the direct problem is

$$u(x,y,t) = \frac{1}{2\pi}\int_{\mathbb{R}^2} e^{-x\sqrt{(i\eta)^{\alpha}+\zeta^2}}\hat{f}(\zeta,\eta)e^{i(\zeta y+\eta t)}d\zeta d\eta. \tag{B-8}$$

We define the operator $K : L^2 \mapsto L^2$ which takes the form

$$[Kf](y,t) = \frac{1}{2\pi}\int_{\mathbb{R}^2} e^{-\sqrt{(i\eta)^{\alpha}+\zeta^2}}\hat{f}(\zeta,\eta)e^{i(\zeta y+\eta t)}d\zeta d\eta = \tag{B-9}$$

$$\frac{1}{2\pi}\int_{\mathbb{R}^2} e^{-\sqrt{(i\eta)^{\alpha}+\zeta^2}}e^{i(\zeta y+\eta t)}\left(\frac{1}{2\pi}\int_{R^2} e^{-i(\zeta\bar{y}+\eta\bar{t})}f(\bar{y},\bar{t})d\bar{y}d\bar{t}\right)d\zeta d\eta = \tag{B-10}$$

$$\int_{\mathbb{R}^2}\left(\frac{1}{4\pi^2}\int_{R^2} e^{-\sqrt{(i\eta)^{\alpha}+\zeta^2}}e^{i(\zeta y+\eta t)}e^{-i(\zeta\bar{y}+\eta\bar{t})}d\zeta d\eta\right)f(\bar{y},\bar{t})d\bar{y}d\bar{t}, \tag{B-11}$$

the term

$$\frac{1}{4\pi^2}\int_{R^2} e^{-\sqrt{(i\eta)^{\alpha}+\zeta^2}}e^{i(\zeta y+\eta t)}e^{-i(\zeta\bar{y}+\eta\bar{t})}d\zeta d\eta \tag{B-12}$$

acts as the kernel of the operator which is wanted to be compact.

Claim.

$$k(y,t,\bar{y},\bar{t}) = \int_{R^2} e^{-\sqrt{(i\eta)^{\alpha}+\zeta^2}}e^{i(\zeta y+\eta t)}e^{-i(\zeta\bar{y}+\eta\bar{t})}d\zeta d\eta \in L^2(\mathbb{R}^2\times\mathbb{R}^2). \tag{B-13}$$

Proof. We will establish first $e^{-\sqrt{(i\eta)^\alpha+\zeta^2}} \in L^2(\mathbb{R}^2)$. We define $\omega = \sqrt{(i\eta)^\alpha + \zeta^2}$ and we can write it in the form $\omega = a + bi$ ([50]), where

$$a = \sqrt{\frac{\sqrt{|\eta|^{2\alpha} sin^2\left(\frac{\alpha\pi}{2}\right) + \left(\zeta^2 + |\eta|^{2\alpha} cos\left(\frac{\alpha\pi}{2}\right)\right)^2} + \left(\zeta^2 + |\eta|^{2\alpha} cos\left(\frac{\alpha\pi}{2}\right)\right)}{2}},$$

$$b = i\ sign\left(sign(\eta) sin\left(\frac{\alpha\pi}{2}\right)\right) \cdot \sqrt{\frac{\sqrt{|\eta|^{2\alpha} sin^2\left(\frac{\alpha\pi}{2}\right) + \left(\zeta^2 + |\eta|^{2\alpha} cos\left(\frac{\alpha\pi}{2}\right)\right)^2} - \left(\zeta^2 + |\eta|^{2\alpha} cos\left(\frac{\alpha\pi}{2}\right)\right)}{2}}.$$

It is important to notice $a \geq 0$ for any η and ζ, providing $\alpha \in (0,1)$, as well as a increasing function of η and ζ. Making use of this fact and that $a(\zeta,\eta) \geq (|\eta|^\alpha \sqrt{cos\left(\frac{\alpha\pi}{2}\right)} + |\zeta|)/2$, we get

$$\int_{R^2} \left| e^{-\sqrt{(i\eta)^\alpha+\zeta^2}} \right|^2 d\zeta d\eta = \int_{R^2} \left| e^{-a-bi} \right|^2 d\zeta d\eta \tag{B-14}$$

$$= \int_{R^2} e^{-2a} d\zeta d\eta \tag{B-15}$$

$$\leq \int_{R^2} e^{-|\eta|^\alpha \sqrt{cos\left(\frac{\alpha\pi}{2}\right)} - |\zeta|} d\zeta d\eta < \infty, \tag{B-16}$$

this implies there exits a function $\Phi \in L^2(\mathbb{R}^2)$ which satisfy $\mathscr{F}\{\Phi\} = e^{-\sqrt{(i\eta)^\alpha+\zeta^2}}$. Since

$$k(y,t,\bar{y},\bar{t}) = \frac{1}{4\pi^2} \int_{R^2} e^{-\sqrt{(i\eta)^\alpha+\zeta^2}} e^{i(\zeta(y-\bar{y})+\eta(t-\bar{t}))} d\zeta d\eta, \tag{B-17}$$

$$= \frac{1}{2\pi} \Phi(y-\bar{y}, t-\bar{t}). \tag{B-18}$$

Finally using the Plancherel's Theorem ([51])

$$\|k(y,t,\bar{y},\bar{t})\|_{L^2}^2 = \frac{1}{2\pi} \|\Phi(y-\bar{y},t-\bar{t})\|_{L^2}^2 = \frac{1}{2\pi} \|e^{-\sqrt{(i\eta)^\alpha+\zeta^2}}\|_{L^2}^2 < \infty$$

□

This fact implies K to be compact because k is a Hilbert-Schmidt kernel. Our initial problem was the inverse one, we want to find f from an observation of g but only have access to a noisy data g^δ. On that direction we establish the minimization problem as follow

$$\underset{f}{\operatorname{argmin}} \left\{ \frac{1}{2} \|Kf - g^\delta\|_{L^2}^2 \right\}. \tag{B-19}$$

This is known to be ill-posed ([50]) and we propose a regularization of it though the Total Variation, then replace the original formulation for the next one

$$\underset{f}{\operatorname{argmin}} \left\{ \frac{1}{2} \|Kf - g^\delta\|_{L^2}^2 + \gamma \int_{\mathbb{R}^2} \sqrt{f_y^2 + f_t^2 + \beta}\, dydt \right\}, \tag{B-20}$$

another regularization parameter is added as in [14] for ensure well behavior of the method. A fixed point method as in [47] will be implemented as below

$$-\gamma \nabla \cdot \left(\frac{\nabla f^{k+1}}{\sqrt{|\nabla f^k|^2 + \beta}} \right) + K^* \left(K f^{k+1} - g^\delta \right) = 0, \tag{B-21}$$

we start with $f^0 = g^\delta$.

Claim.

$$[K^* h](\bar{y}, \bar{t}) = \int_{\mathbb{R}^2} \frac{1}{2\pi} \Phi(y - \bar{y}, t - \bar{t}) h(y,t) dydt \tag{B-22}$$

Proof.

$$\begin{aligned}
\langle Kf, h \rangle &= \int_{\mathbb{R}^2} \left(\int_{\mathbb{R}^2} \frac{1}{2\pi} \Phi(y - \bar{y}, t - \bar{t}) f(\bar{y}, \bar{t}) d\bar{y} d\bar{t} \right) h(y,t) dydt \\
&= \int_{\mathbb{R}^2} \left[\int_{\mathbb{R}^2} \left(\frac{1}{4\pi^2} \int_{R^2} e^{-\sqrt{(i\eta)^\alpha + \zeta^2}} e^{i(\zeta y + \eta t)} e^{-i(\zeta \bar{y} + \eta \bar{t})} d\zeta d\eta \right) f(\bar{y}, \bar{t}) d\bar{y} d\bar{t} \right] h(y,t) dydt \\
&= \int_{\mathbb{R}^2} \left[\int_{\mathbb{R}^2} \left(\frac{1}{4\pi^2} \int_{R^2} e^{-\sqrt{(i\eta)^\alpha + \zeta^2}} e^{i(\zeta y + \eta t)} e^{-i(\zeta \bar{y} + \eta \bar{t})} d\zeta d\eta \right) h(y,t) dydt \right] f(\bar{y}, \bar{t}) d\bar{y} d\bar{t} \\
&= \int_{\mathbb{R}^2} \left(\int_{\mathbb{R}^2} \frac{1}{2\pi} \Phi(y - \bar{y}, t - \bar{t}) h(y,t) dydt \right) f(\bar{y}, \bar{t}) d\bar{y} d\bar{t}
\end{aligned}$$

□

Remark. *From the last proof we notice that K^* is equivalent to take inverse Fourier Transform of h then multiply by $e^{-\sqrt{(i\eta)^\alpha + \zeta^2}}$, and finally take Fourier transform to obtain the result.*

Bibliography

[1] C. D. Acosta, R. Bürger, and C. E. Mejía. Monotone difference schemes stabilized by discrete mollification for strongly degenerate parabolic equations. *Numerical Methods for Partial Differential Equations*, 28(1):38–62, 2012.

[2] C. D. Acosta, R. Bürger, and C. E. Mejía. A stability and sensitivity analysis of parametric functions in a sedimentation model. *DYNA*, 81(183):22–30, 2014.

[3] C. D. Acosta, R. Bürger, and C. E. Mejía. Efficient parameter estimation in a mocroscopic traffic flow model by discrete mollification. *Transportmetrica A: Transport Science*, 11(8):702–715, 2015.

[4] C. D. Acosta and C. E. Mejía. Stabilization of explicit methods for convection diffusion equations by discrete mollification. *Comput. Math. Appl.*, 55:368–380, 2008.

[5] C.D. Acosta and R. Burger. Difference schemes stabilized by discrete mollification for degenerate parabolic equations in two space dimensions. *IMA J. Numer. Anal.*, 32:1509–1540, 2012.

[6] C.D. Acosta and C.E. Mejía. *Stable computations by discrete mollification*. Universidad Nacional de Colombia, 2014.

[7] A. Aldoghaither and T. Laleg-Kirati. Parameter and differentiation order estimation for a two dimensional fractional partial differential equation. *Journal of Computational and Applied Mathematics*, 369:112570, 2020.

[8] E.J. Anderson and M.S. Phanikumar. Surface storage dynamics in large rivers: Comparing three-dimensional particle transport, one-dimensional fractional derivative and multirate transient storage models. *Water Resources Research*, 47:W09511, 2011.

[9] Isaac Asimov. *Asimov's Biographical Encyclopedia Of Science And Technology*. Doubleday, 2nd edition, 1982.

[10] D. Benson, M. Meerschaert, and J. Revielle. Fractional calculus in hydrologic modeling: A numerical perspective. *Advances in Water Resources*, 51:479–497, 2013.

[11] D.A. Benson, S.W. Wheatcraft, and M.M. Meerschaert. Application of a fractional advection-dispersion equation. *Water Resources Research*, 36(6):1403–1412, 2000.

[12] H. Brezis. *Functional Analysis, Sobolev Spaces and Partial Differential Equations*. Universitext. Springer New York, 2010.

[13] R. Brociek, A. Chmielowska, and D. Slota. Comparison of the probabilistic ant colony optimization algorithm and some iteration method in application for solving the inverse problem on model with the caputo type fractional derivative. *Entropy*, 22:555, 2020.

[14] T. Chan, G. Golub, and P. Mulet. A nonlinear primal-dual method for total variation-based image restoration. *SIAM Journal on Scientific Computing*, 20(6):1964–1977, 1999.

[15] K. Diethelm. *The Analysis of Fractional Differential Equations: An Application-Oriented Exposition Using Differential Operators of Caputo Type*. Lecture Notes in Mathematics. Springer Berlin Heidelberg, 2010.

[16] M.D. Echeverry and Mejía C.E. A two dimensional discrete mollification operator and the numerical solution of an inverse source problem. *AXIOMS*, xx,5; doi:10.3390/axiomsxx010005:11, 2018.

[17] S. Fomin and T. Chugunov, V. ahd Hashida. Application of fractional differential equations for modeling the anomalous diffusion of contaminant from fracture into porous rock matrix with bordering alteration zone. *Transport in Porous Media*, 81(2):187–205, Jan 2010.

[18] D. Gilbarg and N.S. Trudinger. *Elliptic Partial Differential Equations of Second Order*. Classics in Mathematics. Springer Berlin Heidelberg, 2001.

[19] R. Gorenflo and F. Mainardi. Fractional calculus: integral and differential equations of fractional order. *arXiv:0885.3823v1*, 2008.

[20] C. Groetsch. *Inverse Problems in the Mathematical Sciences*. Vieweg, 1993.

[21] P. Hansen. *Rank-Deficient and Discrete Ill-Posed Problems*. Society for Industrial and Applied Mathematics, 1998.

[22] P. Hansen. *Discrete inverse problems, insight and algorithms*. SIAM, 2010.

[23] G. Huang, Q. Huang, and H. Zhan et al. Modeling contaminant transport in homogeneous porous media with fractional advection-dispersion equation. *Science in China Ser. D Earth Sciences*, 48(Supp. II):295–302, 2005.

[24] V. Isakov. *Inverse Problems for Partial Differential Equations*. Applied Mathematical Sciences. Springer International Publishing, 2017.

[25] J.C. Lagarias, J.A. Reeds, M.H. Wright, and P.E. Wright. Convergence properties of the nelder-mead simplex method in low dimensions. *SIAM Journal of Optimization*, 9:112–147, 1998.

[26] P. Linz. *Analytical and Numerical Methods for Volterra Equations*. Society for Industrial and Applied Mathematics, 1985.

[27] F. Liu, Anh V.V., I. Turner, and P. Zhuang. Time fractional advection-dispersion equation. *J. Appl. Math. and Computing*, 13:233–245, 2003.

[28] Y. Ma, P. Prakash, and A. Deiveegan. Generalized tikhonov methods for an inverse source problem of the time-fractional diffusion equation. *Chaos, Solitons and Fractals*, 108:39–48, 03 2018.

[29] Agnieszka B. Malinowska, Tatiana Odzijewicz, and Delfim F. M. Torres. *Advanced Methods in the Fractional Calculus of Variations*. Springer Publishing Company, Incorporated, 2015.

[30] M.M. Meerschaert and C. Tadjeran. Finite difference approximations for fractional advection-dispersion flow equations. *Journal of Computational and Applied Mathematics*, 172:65–77, 2004.

[31] C. E. Mejía and A. Piedrahita. Solution of a time fractional inverse advection-dispersion problem by discrete mollification. *Revista Colombiana de Matemáticas*, 51(1):83–102, 2017.

[32] C. E. Mejía and A. Piedrahita. A finite difference approximation of a two dimensional time fractional advection-dispersion problem. *https://arxiv.org/abs/1807.07393*, 2018.

[33] K.S. Miller and B. Ross. *An introduction to the fractional calculus and fractional differential equations*. Wiley, 1993.

[34] D.A. Murio. *The Mollification Method and the Numerical Solution of Ill-Posed Problems*. Wiley, 1993.

[35] P.G. Nutting. A new general law of deformation. *Journal of the Franklin Institute*, 191(5):679 – 685, 1921.

[36] P.G. Nutting. A general stress-strain-time formula. *Journal of the Franklin Institute*, 235(5):513 – 524, 1943.

[37] K.B. Oldham and J. Spanier. *The fractional calculus: theory and applications of differentiation and integration to arbitrary order*. Dover, Mineola, 2006.

[38] I. Podlubny. *Fractional differential equations*. Academic Press, 1999.

[39] A. Saadatmandi and M. Dehghan. A tau approach for solution of the space fractional diffusion equation. *Computers and Mathematics with Applications*, 62(3):1135 – 1142, 2011.

[40] K. Sakamoto and M. Yamamoto. Initial value/boundary value problems for fractional diffusion-wave equations and applications to some inverse problems. *Journal of Mathematical Analysis and Applications*, 382(1):426 – 447, 2011.

[41] S. Salsa. *Partial Differential Equations in Action: From Modelling to Theory*. UNITEXT. Springer International Publishing, 2016.

[42] G. W. Scott Blair and M. Reiner. The rheological law underlying the nutting equation. *Applied Scientific Research*, 2(1):225, Jan 1951.

[43] R. Shikrani and M.S. Hashmi et al. An efficient numerical approach for space fractional partial differential equations. *Alexandria Engineering Journal*, Article in press, 2020.

[44] Martin. Stynes, Eugene. O'Riordan, and José Luis. Gracia. Error analysis of a finite difference method on graded meshes for a time-fractional diffusion equation. *SIAM Journal on Numerical Analysis*, 55(2):1057–1079, 2017.

[45] H. Sun, Y. Zhang, D. Baleanu, and W. Chen. A new collection of real world applications of fractional calculus in science and engineering. *Commun Nonlinear Sci Numer Simulat*, 64:213–231, 2018.

[46] H. Sun, Y. Zhang, D. Baleanu, Chen W., and Chen Y. A new collection of real world applications of fractional calculus in science and engineering. *Commun Nonlinear Sci Numer Simulat*, 64:213–231, 2018.

[47] C. Vogel and M. Oman. Iterative methods for total variation denoising. *SIAM Journal on Scientific Computing*, 17(1):227–238, 1996.

[48] H. Wei, W. Dang, and S. Wei. Parameter identification of solute transport with spatial fractional advection-dispersion equation via tikhonov regularization. *Optik*, 129:8–14, 2017.

[49] R. Weiss and R. S. Anderssen. A product integration method for a class of singular first kind volterra equations. *Numer. Math.*, 18(5):442–456, October 1971.

[50] X. Xiong and X. Xue. Fractional tikhonov method for an inverse time-fractional diffusion problem in 2-dimensional space. *Bulletin of the Malaysian Mathematical Sciences Society*, 2018.

[51] K. Yosida. *Functional Analysis*. Classics in mathematics / Springer. World Publishing Company, 1980.

[52] D. Zhang and G. Li et al. Numerical identification of multiparameters in the space fractional advection dispersion equation by final observations. *Journal of Applied Mathematics*, 2012:740385, 2012.

[53] P. Zhuang and F. Liu. Finite difference approximation for two-dimensional time fractional diffusion equation. *Journal of Algorithms & Computational Technology*, 1(1):1–16, 2007.