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Spectral collocation methods for the fractional PDEs in unbounded domain

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Date of Award:
2018

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HONG KONG BAPTIST UNIVERSITY

Doctor of Philosophy

THESIS ACCEPTANCE

DATE: July 26, 2018

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THESIS TITLE: Spectral collocation Methods for the Fractional PDEs in Unbounded Domain

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Spectral Collocation Methods for the Fractional PDEs in Unbounded Domain

YUAN Huifang

A thesis submitted in partial fulfillment of the requirements
for the degree of
Doctor of Philosophy

Principal Supervisor: Prof. TANG Tao

Hong Kong Baptist University

July 2018

Declaration

I hereby declare that this thesis represents my own work which has been done after registration for the degree of PhD at Hong Kong Baptist University, and has not been previously included in a thesis or dissertation submitted to this or any other institution for a degree, diploma or other qualifications.

I have read the University's current research ethics guidelines, and accept responsibility for the conduct of the procedures in accordance with the University's Committee on the Use of Human & Animal Subjects in Teaching and Research (HASC). I have attempted to identify all the risks related to this research that may arise in conducting this research, obtained the relevant ethical and/or safety approval (where applicable), and acknowledged my obligations and the rights of the participants.

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Date: July 2018

Abstract

This thesis is concerned with a particular numerical approach for solving the fractional partial differential equations (PDEs). In the last two decades, it has been observed that many practical systems are more accurately described by fractional differential equations (FDEs) rather than the traditional differential equation approaches. Consequently, it has become an important research area to study the theoretical and numerical aspects of various types of FDEs. This thesis will explore high order numerical methods for solving FDEs numerically. More precisely, spectral methods which exhibits exponential order of accuracy will be investigated. The method consists of expanding the solution with proper global basis functions and imposing collocation conditions on the Gauss quadrature points.

In this work, Hermite and modified rational functions are employed to serve as basis functions for solutions that decay exponentially and algebraically, respectively. The main emphasis of this thesis is to propose the spectral collocation method for FDEs posed in *unbounded domains*. Components of the differentiation matrix involving fractional Laplacian are derived which can then be computed recursively using the properties of confluent hypergeometric function or hypergeometric function.

The first part of the thesis introduces preliminaries useful for other parts of the thesis. Review of the relevant definitions and properties of special functions such as Hermite functions, Bessel functions, hypergeometric functions, Gegenbauer polynomials, mapped Jacobi polynomials, modified rational functions are presented. Fractional Sobolev space is introduced and some lemmas on interpolation approximation in the fractional Sobolev space are also included.

In the second part of the thesis, we present the spectral collocation method based on Hermite functions. Two bases are used, namely, the over-scaled Hermite function and generalized Hermite function, which are orthogonal functions on the whole line with appropriate weight functions. We will show that the fractional Laplacian of these two kinds of Hermite functions can be represented by confluent hypergeometric function. Behaviors of the condition numbers for the resulting spectral differentiation matrices with respect to the number of expansion terms are investigated.

Moreover, approximation in two-dimensional space using the tensorized bases, application to multi-term problems and use of scaling to match different decay rate are also considered. Convergence analysis for generalized Hermite function are derived and numerical errors for two bases are analyzed.

The third part of the thesis deals with the spectral collocation method based on modified rational functions. We first give a brief introduction for computation of the fractional Laplacian using modified rational functions, which is represented by hypergeometric functions. Then the differentiation matrix involving the fractional Laplace operator is given. Convergence analysis for modified Chebyshev rational functions and modified Legendre rational functions are derived and numerical experiments are carried out.

Keywords: Fractional PDEs, Hermite polynomials/functions, Gegenbauer polynomials, mapped Jacobi functions, modified rational function, unbounded domain, spectral collocation methods.

Acknowledgements

I would like to express my deepest gratitude to my supervisor Prof. Tao Tang for all of his help and encouragement throughout the past four years. It has been a great privilege to work with him. Moreover, I am grateful to Dr. Tao Zhou, Dr. Jiang Yang, and Dr. Bo Gong for discussing research with me, and for giving valuable suggestions. And I appreciate my parents, family members, and friends in HKBU for their caring and support.

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List of Symbols

$C_n^{\lambda}(t)$	Gegenbauer polynomial
$D_{\nu}(x)$	Parabolic cylinder function
${}_1F_1(a;b;x)$	Confluent hypergeometric function
${}_2F_1(a,b;c;x)$	Hypergeometric function
$H_n(x)$	Hermite polynomial
$\widetilde{H}_n(x)$	Over-scaled Hermite function
$\widehat{H}_n(x)$	Generalized Hermite function
$H^s(\mathbb{R})$	Fractional Hilbert space
$I_{\mu}(x)$	Modified Bessel function of the first kind
$\hat{I}_N^h$	Interpolation operator with generalized Hermite function
I_N^{λ}	Interpolation operator with modified rational function
$j_n^{\alpha,\beta}(x)$	Mapped Jacobi polynomial
$J_n^{\alpha,\beta}(t)$	Jacobi polynomial
$J_{\mu}(x)$	Bessel function of the first kind
$K_{\mu}(x)$	Modified Bessel function of the second kind
P_N	Sobolev space of polynomials degree less than or equal to N
$\hat{P}_N$	Span of generalized Hermite function order no bigger than N
V_N^{λ}	Span of modified rational function order no bigger than N

List of Abbreviation

PDEs	Partial differential equations
FPDEs	Fractional partial differential equations
GJFs	Generalized Jacobi functions
DM	Differentiation matrix

Chapter 1

Introduction

1.1 Fractional differential equations

Fractional differential equations are a generalization of differential equations involving derivatives of any arbitrary order, real or complex. The concept of fractional derivative first appeared in a letter to Leibniz by I'Hospital in 1695 asking about what the derivative of order $\frac{1}{2}$ is. And then the foundation of the theory study were laid by Liouville in a paper from 1832. While the integer order derivative of a function at a specific point is a local property, which depends only on values of the function near that point, fractional derivatives involve information of the function further out and are usually defined via singular integral, Fourier or Laplace transform, see [47, 63, 69]. Typical fractional derivatives are Riemann-Liouville fractional derivative, Caputo fractional derivative, Grünwald-Letnikov derivative, Riesz derivative and so on. Common differential equations like advection dispersion equation, diffusion equation, and Schrödinger equation can be rewritten in fractional forms with the corresponding names of fractional advection dispersion equation, fractional diffusion equation and fractional Schrödinger equation where the originally integer order derivatives are replaced with fractional derivatives.

Next we give an example to explain how fractional differential equations are obtained and the major difference from integer ones. Let $\Omega \in \mathbb{R}^d$ be a bounded, open domain, a typical diffusion equation which describes the behavior of the collective motion of micro-particles in a material undergoing diffusion is written as:

$$\begin{cases} \dfrac{\partial \phi\left(x,t\right)}{\partial t} = \bigtriangledown \cdot \left[D\left(\phi,x\right) \bigtriangledown \phi\left(x,t\right)\right] & \text{on } \Omega, \\ \phi\left(x,0\right) = \phi_0 & \text{on } \Omega, \\ \mathcal{B}\phi = g & \text{on } \partial\Omega, \end{cases} \tag{1.1}$$

where $\phi\left(x,t\right)$ is the density of the diffusing material at collocation x and time t and $D\left(\phi,x\right)$ denotes the collective diffusion coefficient for density ϕ at location x. $\mathcal{B}$ denotes a linear operator of constraints acting on the boundary of volume Ω. If D is constant, then the equation reduces to the heat equation. Diffusion equations have found applications in social science material science, information science, and so on. There are many different formulations of the diffusion equation: stochastic model based on Brown motion, physical model based on conservation of mass, and probabilistic model based on central limit theorem. A fundamental result is the linear time dependence of the mean squared displacement, which is characteristic of Brown motion. However, a lot of experimental observations in a wide diversity of systems have found that mean squared displacement scales as a fractional power law in time, which is then called anomalous diffusion. The extension from integer order diffusion equation to fractional differential equations is among the many efforts to deal with this phenomenon. Fractional diffusion equations are obtained by replacing the space derivative or time derivative with fractional derivatives. For example, with fractional spatial differential operators, the following fractional diffusion problem can be defined.

$$\begin{cases} \dfrac{\partial \phi\left(x,t\right)}{\partial t} = \mathcal{L}\phi\left(x,t\right) & \text{on } \Omega, \\ \phi\left(x,0\right) = \phi_0 & \text{on } \Omega \cup \Omega_I, \\ \mathcal{V}\phi = g & \text{on } \Omega_I, \end{cases} \tag{1.2}$$

where $\mathcal{V}$ denotes a linear operator of constraints acting on the the volume Ω_I that is disjoint from Ω. Here $\mathcal{L}$ is a fractional differential operator with respect to x and a generalization of the second-order elliptic derivative $\bigtriangledown \cdot \left(D\left(\phi,x\right) \bigtriangledown\right)$. For example, when dimension $d = 1$, $\Omega_I = \mathbb{R}\backslash\Omega$, and $D\left(\phi,x\right)$ is constant, the following Riesz fractional derivative with $1 < \alpha < 2$ is defined as:

$$\frac{\partial^\alpha}{\partial |x|^\alpha}\phi\left(x\right) = \frac{{}^{RL}_{-\infty}D^\alpha_x\phi\left(x\right) + {}^{RL}_{x}D^\alpha_\infty\phi\left(x\right)}{2\cos\left(\alpha\pi/2\right)},$$

where ${}^{RL}_{-\infty}D^{\alpha}_{x}$ and ${}^{RL}_{x}D^{\alpha}_{\infty}$ represents the left and right Rieman-Liouville fractional derivative defined by

$$
\begin{aligned}
{}^{RL}_{-\infty}D^{\alpha}_{x}\phi(x) &= \frac{1}{\Gamma(2-\alpha)}\frac{\partial^2}{\partial x^2}\int_{-\infty}^{x}\frac{\phi(\xi)}{(x-\xi)^{\alpha-1}}d\xi,\\
{}^{RL}_{x}D^{\alpha}_{\infty}\phi(x) &= \frac{1}{\Gamma(2-\alpha)}\frac{\partial^2}{\partial x^2}\int_{x}^{\infty}\frac{\phi(\xi)}{(\xi-x)^{\alpha-1}}d\xi.
\end{aligned}
$$

The main difference between the above two diffusion problems (1.1) and (1.2) are twofolds: First, the second order spatial differential operator $\bigtriangledown\cdot(D(\phi,x)\bigtriangledown)$ is replaced with fractional derivative $\mathcal{L}$. Secondly, in (1.1), the linear constraints are pose on the boundary surface, while in (1.2) constraints are on a nonzero volume Ω_I. Numerical study of fractional diffusion equations of this form can be found in [22, 23, 24, 70, 92]. At the same time, it is also possible to replace the first order time derivative with fractional operators, for example, Caputo derivatives. As demonstrated before, in fractional diffusion mean squared displacement scales as a fractional power law in time. If the fractional power is less than unity, then the fractional diffusion is referred to as subdiffusion and superdiffusion for fractional power greater than unity. Fractional diffusion is universal and has been found in spatially disordered systems, turbulent fluids and plasmas, and in biological media with traps. Other applications of fractional differential equations include fractional advection-dispersion equation characterizing the collective behavior of partical transport on the earth surface, see in [6, 72], the fractional Schrödinger equation in fractional quantum mechanics, see in [49, 80], and many other forms. Mathematical modeling for fractional differential equations can be obtained by continuous time random walk, the generalized central limit theorem and others, see in [18, 37, 56, 83].

1.2 Numerical methods

Progress in the past two decades has demonstrated that many phenomena in science, economics, and engineering are more accurately described by fractional differential equations (FDEs) rather than the traditional approaches [7, 8, 61] due to their unique capacity in description of long-range time memory and spatial interactions. And this leads to a lot theoretical studies, for example, boundary conditions in [4, 20, 25, 29], and regularity results in [2, 60, 68, 71]. At the same time, the analytic solutions of the FPDEs are usually unknown or derived via Green functions and Fox functions that are difficult to evaluate. So there has been an intensive investigation over the past two decades on efficient numerical methods for FPDEs. Among others, the finite difference method and the finite element method are two widely investigated methods in this direction, see, e.g., [38, 40, 41, 46, 66, 81, 90] and references therein. However the extension from integer order differential equations to fractional order ones is nontrivial because of the nonlocal property of the fractional differential operators. In particular, finite difference/element methods lead to full and dense matrices that are expensive to calculate and invert.

Another powerful approach is the spectral method, which is natural for the nonlocal feature of the fractional operators, since spectral method is global. In this approach, the key is to construct suitable basis functions to handle to the solution singularities. Along this direction, a recent advance is brought by Zayernouri and Karniadakis who proposed the so-called Jacobi *poly-fractonomials* based spectral methods [93]. These bases are eigenfunctions of the corresponding fractional and tempered fractional Sturm-Liouville problems. Another approach that employs the generalized Jacobi functions (GJFs) is proposed by Shen et al. [17]. Those bases are adapted to the fractional operator, as a fractional derivative of poly-fractonomials/GJFs is simply another poly-fractonomials/GJFs with different parameters. Consequently, fractional derivatives become a local operator in the physical space spanned by poly-fractonomials/GJFs, and this property leads to very efficient spectral methods for fractional PDEs in bounded domains. The poly-fractonomials/GJFs have been successfully applied to various fractional models [16, 43, 52]. However, compared to fractional PDEs in bounded domain, little works have been done for fractional PDEs defined on unbounded domains. Very recently, spectral methods for fraction differential equations in the half line are proposed in [44, 52] – using the generalized Laguerre functions as bases – extending the idea of [93]. Also Mao and Shen [54] proposed both the spectral Galerkin and collocation method for fractional PDEs in unbounded domains. However, the collocation method therein relies on an equivalent formulation in frequency space by the Fourier transform, and performs collocation methods to the equivalent formulation that involve forward/backward Hermite transform.

1.3 Problem description

In this thesis, we shall concentrate on designing spectral collocation methods for fractional PDEs in unbounded domains (the whole space $\mathbb{R}^d$). To better demonstrate our idea, we consider the following model equation:

$$\begin{cases} (-\Delta)^{\alpha/2} u(x) + \rho u(x) = f(x), & x \in \mathbb{R}^d, \\ u(x) = 0, & |x| \to \infty, \end{cases} \tag{1.3}$$

where $\rho \geq 0$, $0 < \alpha < 2$. Notice that the above fractional differential equation is obtained by replacing the second-order Laplace operator $(-\Delta)$ with the fractional Laplacian of order α, which recovers the standard Laplace operator as $\alpha \to 2$.

The properties and general numerical treatment of fractional Laplacian has been studied in [12, 64]. There are numerous ways to define the fractional Laplace operator in bounded and unbounded domain. In unbounded domain, the fractional Laplacian of order α, $0 < \alpha < 2$ can be defined by

- Singular integral[48]

$$(-\Delta)^{\alpha/2}u(x) = C_{d,\alpha}\text{P.V.} \int_{\mathbb{R}^d} \frac{u(x)-u(y)}{|x-y|^{d+\alpha}}dy, \quad \text{with} \quad C_{d,\alpha} = \frac{\alpha 2^{\alpha-1}\Gamma\left(\frac{\alpha+d}{2}\right)}{\pi^{d/2}\Gamma\left(\frac{2-\alpha}{2}\right)}. \tag{1.4}$$

  The "P.V." denotes the principle value of the integral:

$$\text{P.V.} \int_{\mathbb{R}^d} \frac{u(x)-u(y)}{|x-y|^{d+\alpha}}dy = \lim_{\epsilon\to 0} \int_{\mathbb{R}^d \setminus B_\epsilon} \frac{u(x)-u(y)}{|x-y|^{d+\alpha}}dy$$

  where B_ϵ is a ball of radius ϵ. The numerator $u(x) - u(y)$ of (1.4) which averages out in a neighborhood of x by symmetry allows the existence of principle value for smooth u with sufficient decay rate. It is easy to verify the asymptotic behavior for $C_{d,\alpha}$: as $\alpha \to 0$, $C_{d,\alpha} \approx \frac{\alpha\Gamma(d/2)}{2\pi^{d/2}}$ and as $\alpha \to 2$, $C_{d,\alpha} \approx \frac{d\Gamma(d/2)}{\pi^{d/2}}(2-\alpha)$. In both cases α tends to 0.

- Fourier transform:

$$\mathcal{F}\left[(-\Delta)^{\alpha/2}u\right](\xi) = |\xi|^\alpha \mathcal{F}[u](\xi). \tag{1.5}$$

where the Fourier transform $\mathcal{F}[u]$ of a function $u : \mathbb{R}^d \to \mathbb{R}$ is given by

$$\mathcal{F}[u]\,(\xi) = \int_{\mathbb{R}^d} u(x) e^{-ix\cdot\xi} dx.$$

The definition in (1.5) provides a simple method for solving problems like $(-\Delta)^{\alpha/2} u\,(x) = f\,(x)$ assuming f decays fast enough in infinity.

- The heat semigroup. Recall the numerical formula

$$\lambda^s = \frac{1}{\Gamma\,(-s)} \int_0^\infty \left(e^{-t\lambda} - 1\right) \frac{dt}{t^{1+s}},$$

valid for $\lambda \geq 0$ and $0 < s < 1$. By taking $\lambda = |\xi|^2$ and using the Fourier transform definition of the fractional Laplacian in (1.5) we have

$$(-\Delta)^{\alpha/2} u(x) = \frac{1}{\Gamma\left(-\frac{\alpha}{2}\right)} \int_0^\infty \left(e^{t\Delta} u\,(x) - u\,(x)\right) \frac{dt}{t^{1+\alpha/2}}.$$

Details of the definition by heat semigroup can be found in [76, 77].

- As a generator of a Levy process. The fractional Laplacian is connected to anomalous diffusion which has received a lot attention to describe many physical scenarios, most prominently within crowded systems. Just as the Laplacian is the negative generator of Brownian motion $B_t = X_t^2$, the fractional Laplacian represents the infinitesimal generator of a symmetric α-stable Lévy process. More precisely, if X_t^α is the isotropic α-stable process in which the increments are drawn from a symmetric α-stable distribution, then

$$(-\Delta)^{\alpha/2} u(x) = \lim_{h \to 0} \frac{1}{h} \mathbb{E}\left[u(x) - u\left(x + X_h^\alpha\right)\right].$$

Details can be found in [51, 55].

These definitions in unbounded domain are equivalent. For example, to prove the equivalent of (1.4) and (1.5), notice that (1.4) can be written in a more compact form:

$$(-\Delta)^{\alpha/2} u(x) = \frac{C_{d,\alpha}}{2} \int_{\mathbb{R}^d} \frac{2u\,(x) - u\,(x-y) - u\,(x+y)}{|y|^{d+\alpha}} dy. \tag{1.6}$$

This provide a simple way to prove the equivalence. Apply Fourier transform to (1.6)

$$\begin{aligned}
\mathcal{F}\left[(-\Delta)^{\alpha/2} u\right](\xi) &= \frac{C_{d,\alpha}}{2} \int_{\mathbb{R}^d} \frac{\mathcal{F}[2u\,(x) - u\,(x-y) - u\,(x+y)]}{|y|^{d+\alpha}} dy \\
&= \frac{C_{d,\alpha}}{2} \int_{\mathbb{R}^d} \mathcal{F}u\,(\xi)\, \frac{2 - e^{i\xi\cdot y} - e^{-i\xi\cdot y}}{|y|^{d+\alpha}} dy \\
&= C_{d,\alpha} \mathcal{F}u\,(\xi) \int_{\mathbb{R}^d} \frac{1 - \cos\left(\xi \cdot y\right)}{|y|^{d+\alpha}} dy.
\end{aligned}$$

Then the equivalence can be obtained by proving

$$C_{d,\alpha}\int_{\mathbb{R}^d}\frac{1-\cos\left(\xi\cdot y\right)}{|y|^{d+\alpha}}dy=|\xi|^{\alpha}$$

More definitions for fractional Laplacian in unbounded domain and proof of their equivalence can be found in [45].

In bounded domain, the study of fractional Laplacian becomes more complicated. Different representations, for example, the Riesz definition, the directional definition or the spectral definition, may lead to different operators when restricted to a bounded domain. Here we give a brief introduction of the spectral decomposition definition on a bounded domain $D\subset\mathbb{R}^d$. Let $\left\{\lambda_k,\phi_k\right\}_k$ be the eigenvalues and eigenfunctions of the negative Laplace operator, i.e.,

$$\left(-\Delta\right)\phi_k\left(x\right)=\lambda_k\phi_k\left(x\right),$$

subject to appropriate boundary conditions that ensure all $\{\lambda_k\}$ are nonnegative and $\{\phi_k\}$ form a complete orthonormal basis. Then if we assume $u\left(x\right)$ has the expansion $u\left(x\right)=\sum_k c_k\phi_k\left(x\right)$, the fractional Laplacian of $u\left(x\right)$ is defined by

$$\left(-\Delta\right)^{\alpha/2}u\left(x\right)=\sum_k c_k\lambda_k^{\alpha/2}\phi_k\left(x\right).$$

More definitions for bounded domain can be found in [51]. Although difference exists among different definitions of fractional Laplacian in unbounded domian, most of these definitions formally converge to fractional Laplacian in $\mathbb{R}^d$ as the domain is extended to the whole space.

Then we look at some simple properties of the fractional Laplace operator. Besides the general properties of fractional derivatives, the fractional Laplacian has the following properties:

- Maximum principle. If u has a global maximum at a point x, then $\left(-\Delta\right)^{\alpha/2}u\left(x\right)\geq 0$, with equality only if u is a constant function. This property can be easily proved by the singular definition in (1.4). From this property, a comparison principle can be derived for equations involving the fractional Laplace operator.

- The semigroup property. By the Fourier transform definition in (1.5), the semigroup property of fractional Laplacian can be easily proved which states

$$(-\Delta)^{\alpha}\Big\{(-\Delta)^{\beta}u(x)\Big\} = (-\Delta)^{\alpha+\beta}u(x).$$

- Scaling property. Let the fractional Laplacian of $v\left(x\right)$ be $\phi\left(x\right)$, i.e.,

$$(-\Delta)^{\alpha/2}v\left(x\right) = \phi\left(x\right),$$

  Then the fractional Laplacian of $v_r\left(x\right) = v\left(rx\right)$ is

$$(-\Delta)^{\alpha/2}v_r\left(x\right) = r^{\alpha}\phi\left(rx\right).$$

  This can be simply proved by using either the definition (1.4) or (1.5).

- Integration by part. For any $v \in C_c^{\infty}\left(\mathbb{R}^d\right)$,

$$\int_{\mathbb{R}^d}(-\Delta)^{\alpha/2}u\left(x\right)v\left(x\right)dx = \int_{\mathbb{R}^d}u\left(x\right)(-\Delta)^{\alpha/2}v\left(x\right)dx.$$

  Moreover, for u, v in proper spaces, we have

$$\left((-\Delta)^{\alpha}u\left(x\right), v\left(x\right)\right) = \Big((-\Delta)^{\alpha/2}u\left(x\right), (-\Delta)^{\alpha/2}v\left(x\right)\Big).$$

The major issue in dealing with the above equation (1.3) is the treatment of the nonlocal fractional Laplace operator which involves a singular kernel and incorporates long range space interactions, and contrary to the classical Laplace operator, where theoretical properties and numerical methods are fully understood. Here are finite difference method in [26, 28, 38] and the references therein. Special care are needed in dealing with the singularity part and far field boundary conditions. In [38], a finite difference/quadature discretization of the fractional Laplacian based on (1.4) was presented with special treatment of the far filed boundary condition. It was proved that $O\left(h^{2-\alpha}\right)$ and $O\left(h^{2-\alpha}\right)$ accuracy are obtained for piecewise linear and quadratic interpolation respectively. In [26], the α-dependence of accuracy is overcomed by introducing a proper splitting parameter and reformulate fractional Laplacian as the weighted integral of a weaker singular function, achieving the accuracy of $O\left(h^2\right)$.

Another approach is α harmonic extension of the fractional Laplacian considered by Caffarelli-Silvestre in [13]. The idea of the extension procedure is that the nonlocal fractional Laplacian operator $(-\Delta)^{\alpha/2}$ defined on $\mathbb{R}^d$ can be reduced to a local operator posed on one more dimension $\mathbb{R}_+^{d+1} := \mathbb{R}^d \times (0, \infty)$. Indeed, take $U : \mathbb{R}_+^{d+1} \to \mathbb{R}$ with $U(x, 0) = u(x)$, solution to the equation

$$\triangledown \cdot \left(y^{1-\alpha} \triangledown U(x, y)\right) = 0, \text{ in } \mathbb{R}_+^{d+1},$$

then up to constants we have

$$(-\Delta)^{\alpha/2} u(x) = -\lim_{y \to 0} \left(y^{1-\alpha} \partial_y U(x, y)\right).$$

Other extension problems for fractional Laplacian and generalizations of other differential operators can be found in [5, 58, 59, 78].

In this thesis, we propose spectral methods for (1.3). Spectral methods have been exclusively studied in [74, 75]. And in [73], Shen and Wang present a systematic framework for spectral methods using mapped Jacobi polynomial, Laguerre and Hermite function. Convergence rate for solutions with typical decay behavior was compared both theoretically and computationally. Here we propose spectral collocation method to handle the fractional differential equation in (1.3). It follows the standard procedure of spectral collocation methods: first expanding the solution with the basis functions and then imposing collocation conditions on the proper Guass quadrature points. In particular, we shall consider two types of expansion bases, that is, the Hermite functions and modified rational function for solutions that decay exponentially and algebraically in infinity, respectively. For both approaches, we shall derive explicit formulas for the associated differential matrix (DM), for which the components can be computed efficiently by using a recurrence formula.

1.4 Plan of the thesis

The rest of the thesis is organized as follows. We provide some preliminaries in next chapter. In Chapter 3, we propose the spectral collocation method based on Hermite functions for solutions that decay exponentially in infinity. Methods based on modified rational functions are considered in Chapter 4 for solutions that decay algebraically in infinity. In both chapters, convergence analysis and numerical examples are presented. We finally give some concluding remarks in Chapter 5.

Chapter 2

Preliminaries

Before presenting our spectral collocation methods, we begin with some preliminary definitions, relations and lemmas that will be useful for the remaining chapters.

2.1 Confluent hypergeometric functions

We first introduce the definition of confluent hypergeometric function of the first kind which is defined in [30] by the following power series

$$ {}_1F_1\left(a;b;x\right) = \sum_{k=0}^{\infty} \frac{(a)_k}{(b)_k} \frac{x^k}{k!}, \tag{2.1} $$

where $(a)_k$ is the Pochhammer symbol defined as

$$ (a)_0 = 1, \quad (a)_k = a\left(a+1\right)\left(a+2\right)...\left(a+k-1\right), k \geq 1. $$

By the above definition, we can easily get the derivative of confluent hypergeometric as

$$ \frac{d^k}{dx^k} {}_1F_1\left(a;b;x\right) = \frac{(a)_k}{(b)_k} {}_1F_1\left(a+k;b+k;x\right). $$

At the same time, confluent hypergeometric can be defined by the following integral representation as in [39]

$$ {}_1F_1\left(a;b;x\right) = \frac{\Gamma\left(b\right)}{\Gamma\left(b-a\right)\Gamma\left(a\right)} \int_0^1 e^{tx} t^{a-1} \left(1-t\right)^{b-a-1} dt, \quad a,\, b > 0. \tag{2.2} $$

It is noticed that the confluent hypergeometric function satisfies the Kummer's transformation formula

$$ {}_1F_1\left(a;b;-x\right) = e^{-x} {}_1F_1\left(b-a;b;x\right). \tag{2.3} $$

Meanwhile, the following recurrence formula holds

$$(2a-b+x)\,{}_1F_1\left(a;b;x\right)=a\,{}_1F_1\left(a+1;b;x\right)-(b-a)\,{}_1F_1\left(a-1;b;x\right). \tag{2.4}$$

2.2 An integral involving parabolic cylinder function

$D_\nu\left(x\right)$ is the parabolic cylinder function defined via confluent hypergeometric function as:

$$D_\nu\left(x\right)=2^{\frac{\nu}{2}}e^{-\frac{x^2}{4}}\left\{\frac{\Gamma\left(\frac{1}{2}\right)}{\Gamma\left(\frac{1-\nu}{2}\right)}{}_1F_1\left(-\frac{\nu}{2};\frac{1}{2};\frac{x^2}{2}\right)+\frac{x}{\sqrt{2}}\frac{\Gamma\left(-\frac{1}{2}\right)}{\Gamma\left(-\frac{\nu}{2}\right)}{}_1F_1\left(\frac{1-\nu}{2};\frac{3}{2};\frac{x^2}{2}\right)\right\}. \tag{2.5}$$

For $0<\nu<1$, we introduce the following integral formula as demonstrated in [30]:

$$\int_0^\infty x^{\nu-1}e^{-\beta x^2-\gamma x}dx=(2\beta)^{-\frac{\nu}{2}}\Gamma\left(\nu\right)\exp\left(\frac{\gamma^2}{8\beta}\right)D_{-\nu}\left(\frac{\gamma}{\sqrt{2\beta}}\right),\, Re(\beta)>0, Re(\nu)>0, \tag{2.6}$$

This equation will be used in next chapter for the derivation of the fractional Laplacian of Hermite functions.

2.3 Hermite polynomials/functions

The Hermite polynomials, denoted by $H_n\left(x\right)$, $n\geqslant 0$, $x\in\mathbb{R}$, are defined by the following three-term recurrence relation (see e.g., [74, 86]):

$$H_0(x)=1,\quad H_1(x)=2x,\quad H_{n+1}(x)=2xH_n(x)-2nH_{n-1}(x),\quad n\geq 1.$$

The Hermite polynomials are orthogonal with respect to the weight function $\omega\left(x\right)=e^{-x^2}$, namely,

$$\int_{\mathbb{R}}H_m(x)H_n(x)e^{-x^2}dx=\gamma_n\delta_{mn},\quad \gamma_n=\sqrt{\pi}2^n n!,$$

and satisfy

$$H_n^{'}(x)=2nH_{n-1}(x).$$

Moreover Hermite polynomial $H_n(x)$ is even when n is an even number, and odd for odd n, i.e.,

$$H_n(-x)=\left(-1\right)^n H_n(x).$$

It is well known that Hermite polynomials and the confluent hypergeometric function satisfy the following formulas:

$$H_{2n}(x) = (-1)^n \frac{(2n)!}{n!} {}_1F_1\left(-n; 1/2; x^2\right); \tag{2.7}$$

$$H_{2n+1}(x) = (-1)^n \frac{(2n+1)!}{n!} 2x {}_1F_1\left(-n; 3/2; x^2\right). \tag{2.8}$$

The corresponding generalized Hermite functions are defined as

$$\widehat{H}_n(x) = \frac{1}{\sqrt{2^n n!}} e^{-x^2/2} H_n(x). \tag{2.9}$$

They are orthogonal with respect to the weight function $\hat{\omega}(x) = 1$, i.e.,

$$\int_{\mathbb{R}} \widehat{H}_m(x) \widehat{H}_n(x) dx = \sqrt{\pi} \delta_{mn}.$$

We shall also discuss the *over-scaled* Hermite bases defined as follows

$$\widetilde{H}_n(x) = \frac{1}{\sqrt{2^n n!}} e^{-x^2} H_n(x). \tag{2.10}$$

It is easy to see that the generalized Hermite defined here is orthogonal with respect to the weight function $\tilde{\omega}(x) = e^{x^2}$, i.e.,

$$\int_{\mathbb{R}} \widetilde{H}_m(x) \widetilde{H}_n(x) e^{x^2} dx = \sqrt{\pi} \delta_{mn}.$$

Such bases were first proposed by Brinkman in [11] and have been well studied in physics, see e.g., [67]. The above over-scaled basis was first proposed when studying the so-called Fokker-Planck equations, where the velocity part of the probability distribution function was expanded in Hermite functions (2.10). This approach has become one of the most popular methods used for solving the Fokker-Planck equation, see, e.g., [27, 67]. We shall discuss the spectral collocation methods based on the above Hermite functions in Chapter 2.

2.4 Bessel functions

We shall also use properties of Bessel functions. Recall that the Bessel function of the first kind of order μ is defined as

$$J_\mu(x) = \sum_{m=0}^{\infty} \frac{(-1)^m}{m!\,\Gamma(m+\mu+1)} \left(\frac{x}{2}\right)^{2m+\mu}. \tag{2.11}$$

In particular we have

$$J_{-\frac{1}{2}}(x) = \sqrt{\frac{2}{\pi x}} \cos x, \qquad J_{\frac{1}{2}}(x) = \sqrt{\frac{2}{\pi x}} \sin x. \tag{2.12}$$

For the Bessel functions it holds in [30] that

$$\int_{\mathbb{R}^+} J_\mu(bt) \exp(-p^2 t^2) t^{\nu-1} dt = \frac{\left(\frac{b}{2p}\right)^\mu \Gamma(\frac{\mu+\nu}{2})}{2p^\nu \Gamma(\mu+1)} {}_1F_1\left(\frac{\mu+\nu}{2}; \mu+1; -\frac{b^2}{4p^2}\right). \tag{2.13}$$

It is easy to check that for Bessel function with integer parameter it holds

$$\frac{d}{dx}\left\{x^{-n} J_n(x)\right\} = -x^{-n} J_{n+1}(x). \tag{2.14}$$

Then we introduce an integral formula involving two Bessel functions. Let m, n be two integers, and let $\nu \geq -n-1,\ \mu \geq -m-1$ be two real numbers, we denote

$$\mu + \nu + m + n := \delta; \quad \mu + \nu - m - n := \zeta. \tag{2.15}$$

Then for $a > 0$ it holds (see e.g, [65], P.216)

$$\begin{aligned} &\int_0^a x^{v+2n+1} \left(a^2 - x^2\right)^{m+\mu/2} J_\mu\left(b\sqrt{a^2-x^2}\right) J_v(cx) dx \\ &= a^{\zeta+1} b^\mu c^v \left(\tfrac{\partial}{b\partial b}\right)^m \left(\tfrac{\partial}{c\partial c}\right)^n \left[\left(b^2+c^2\right)^{-\frac{\delta+1}{2}} J_{\delta+1}\left(a\sqrt{b^2+c^2}\right)\right]. \end{aligned} \tag{2.16}$$

We shall also use in later chapters the modified Bessel function of the first and second kind defined by

$$\begin{aligned} I_\mu(x) &= i^{-\mu} J_\mu(ix) = \sum_{m=0}^{\infty} \frac{1}{m!\,\Gamma(m+\mu+1)} \left(\frac{x}{2}\right)^{2m+\mu}, \\ K_\mu(x) &= \frac{\pi}{2} \frac{I_{-\mu}(x) - I_\mu(x)}{\sin(\mu\pi)}. \end{aligned} \tag{2.17}$$

For the modified Bessel functions of the second kind $K_\mu(x)$ the following integrals hold in [30]:

$$\begin{aligned} \int_0^\infty x^\lambda K_\mu(ax)\cos(bx)dx = \frac{2^{\lambda-1}\Gamma\left(\frac{\mu+\lambda+1}{2}\right)\Gamma\left(\frac{1+\lambda-\mu}{2}\right)}{a^{\lambda+1}} {}_2F_1\left(\frac{\mu+\lambda+1}{2}, \frac{1+\lambda-\mu}{2}; \frac{1}{2}; -\frac{b^2}{a^2}\right), \\ Re\,(-\lambda \pm \mu) < 1, Re a > 0, b > 0; \end{aligned} \tag{2.18}$$

$$\begin{aligned} \int_0^\infty x^\lambda K_\mu(ax)\sin(bx)dx = \frac{2^\lambda b\Gamma\left(\frac{\mu+\lambda+2}{2}\right)\Gamma\left(\frac{2+\lambda-\mu}{2}\right)}{a^{\lambda+2}} {}_2F_1\left(\frac{\mu+\lambda+2}{2}, \frac{2+\lambda-\mu}{2}; \frac{3}{2}; -\frac{b^2}{a^2}\right), \\ Re\,(-\lambda \pm \mu) < 2, Re a > 0, b > 0. \end{aligned} \tag{2.19}$$

Here ${}_2F_1$ is the hypergeometric function which we will introduce in the next section.

2.5 Hypergeometric function

We introduce the hypergeometric function which is defined by the following power series:

$$ {}_2F_1\left(a,b;c;x\right)=\sum_{k=0}^{\infty}\frac{\left(a\right)_k\left(b\right)_k}{\left(c\right)_k}\frac{x^k}{k!}, $$

for $|x|<1$, and by analytic continuation elsewhere. Here $\left(a\right)_k$ is the rising Pochhammer symbol as defined in previous section. By the above definition, we can easily get

$$ \frac{d^k}{dx^k}{}_2F_1\left(a,b;c;x\right)=\frac{\left(a\right)_k\left(b\right)_k}{\left(c\right)_k}{}_2F_1\left(a+k,b+k;c+k;x\right). $$

Hypergeometric function can also be defined by the following integral formula:

$$ {}_1F_1\left(a,b;c;x\right)=\frac{\Gamma\left(b\right)\Gamma\left(c-b\right)}{\Gamma\left(c\right)}\int_0^1 t^{b-1}\left(1-t\right)^{c-b-1}\left(1-tx\right)^{-a}dt,\quad a,\ b>0. $$

Many of the common mathematical functions can be expressed in terms of the hypergeometric function, or as limiting cases of it. One typical example is

$$ {}_2F_1\left(a,b;a;x\right)=\left(1-x\right)^{-b}. \tag{2.20} $$

Also it has the recursion relations for

$$ {}_2F_1\left(a\pm 1,b;c;x\right),\quad {}_2F_1\left(a,b\pm 1;c;x\right),\quad {}_2F_1\left(a,b;c\pm 1;x\right) \tag{2.21} $$

for example, in [30] it holds that

$$ \begin{aligned} &\left(2a-c-ax+bx\right){}_2F_1\left(a,b;c;x\right)+\left(c-a\right){}_2F_1\left(a-1,b;c;x\right)\\ &\qquad\qquad +a\left(x-1\right){}_2F_1\left(a+1,b;c;x\right)=0. \end{aligned} \tag{2.22} $$

With $n=0,1,2,...$, we have the following linear transformation

$$ {}_2F_1\left(-n,b;c;x\right)=\frac{\left(c-b\right)_n}{\left(c\right)_n}{}_2F_1\left(-n,b;b-c-n+1;1-x\right). \tag{2.23} $$

For hypergeometric functions, the following integral formula in [30] hold:

$$ \begin{aligned} &\int_0^{\infty}\cos\left(\mu x\right){}_2F_1\left(\alpha,\beta;\frac{1}{2};-c^2x^2\right)dx=2^{-\alpha-\beta+1}\pi c^{-\alpha-\beta}\mu^{\alpha+\beta-1}\frac{K_{\alpha-\beta}\left(\frac{\mu}{c}\right)}{\Gamma\left(\alpha\right)\Gamma\left(\beta\right)},\\ &\qquad\qquad \mu>0, Re\alpha>0, Re\beta>0, c>0; \end{aligned} \tag{2.24} $$

$$ \begin{aligned} &\int_0^{\infty}x\sin\left(\mu x\right){}_2F_1\left(\alpha,\beta;\frac{3}{2};-c^2x^2\right)dx=2^{-\alpha-\beta+1}\pi c^{-\alpha-\beta}\mu^{\alpha+\beta-2}\frac{K_{\alpha-\beta}\left(\frac{\mu}{c}\right)}{\Gamma\left(\alpha\right)\Gamma\left(\beta\right)},\\ &\qquad\qquad \mu>0, Re\alpha>\frac{1}{2}, Re\beta>\frac{1}{2}. \end{aligned} \tag{2.25} $$

2.6 Gegenbauer polynomials

Jacobi polynomials $J_n^{\alpha,\beta}(t)$, $t \in (-1,1)$, are defined by

$$(1-t)^{\alpha}(1+t)^{\beta} J_n^{\alpha,\beta}(t) = \frac{(-1)^n}{2^n n!}\partial_t^n \left((1-t)^{n+\alpha}(1+t)^{n+\beta}\right).$$

They satisfy the derivative relation

$$\partial_t J_n^{\alpha,\beta}(t) = \frac{1}{2}(n+\alpha+\beta+1) J_{n-1}^{\alpha+1,\beta+1}(t). \tag{2.26}$$

Jacobi polynomials can also be defined by hypergeometric function as follow:

$$J_n^{\alpha,\beta}(t) = \frac{(\alpha+1)_n}{n!}{}_2F_1\left(-n, n+\alpha+\beta+1; \alpha+1; \frac{1-t}{2}\right). \tag{2.27}$$

Gegenbauer polynomials or ultraspherical polynomials $C_n^{\lambda}(t)$ are special cases of Jacobi polynomials with the two parameters being equal, and thus generalize Legendre polynomials and Chebyshev polynomials.

$$C_n^{\lambda}(t) = \frac{(2\lambda)_n}{\left(\lambda+\frac{1}{2}\right)_n} J_n^{(\lambda-1/2,\lambda-1/2)}(t), \quad \lambda > -\frac{1}{2}. \tag{2.28}$$

They satisfy the following three-term recurrence relation:

$$\begin{aligned} &C_0^{\lambda}(t) = 1,\ C_1^{\lambda}(t) = 2\lambda t, \\ &nC_n^{\lambda}(t) = 2t(n+\lambda-1)C_{n-1}^{\lambda}(t) - (n+2\lambda-2)C_{n-2}^{\lambda}(t), n \geq 2. \end{aligned} \tag{2.29}$$

Moreover Gegenbauer polynomials $C_n^{\lambda}(t)$ is even when n is an even number, and odd for odd n, i.e.,

$$C_n^{\lambda}(-t) = (-1)^n C_n^{\lambda}(t).$$

Special values for $t = \pm 1$ are

$$C_n^{\lambda}(1) = \frac{(2\lambda)_n}{n!}, \quad C_n^{\lambda}(-1) = (-1)^n \frac{(2\lambda)_n}{n!}.$$

As for Jacobi polynomials in (2.26), derivatives of Gegenbauer polynomials satisfy

$$\partial_t C_n^{\lambda}(t) = 2\lambda C_{n-1}^{\lambda+1}(t), \text{ for } n \geq 1. \tag{2.30}$$

The Gegenbauer polynomial are eigenfunctions of the following singular Sturm-Liouville problem

$$\partial_t\left(\left(1-t^2\right)^{\lambda+\frac{1}{2}}\partial_t v(t)\right) + n(n+2\lambda)\left(1-t^2\right)^{\lambda-1/2} v(t) = 0,\ t \in (-1,1).$$

They satisfy the orthogonality relation with respect to the weight function $\omega^{\lambda}(t) = (1-t^2)^{\lambda-1/2}$ as:

$$\int_{-1}^{1} \left(1-t^2\right)^{\lambda-1/2} C_n^{\lambda}(t)\, C_m^{\lambda}(t)\, dt = \gamma_n^{\lambda}\delta_{nm}, \quad \gamma_n^{\lambda} = \frac{\pi 2^{1-2\lambda}\Gamma(n+2\lambda)}{n!\,(n+\lambda)\left[\Gamma(\lambda)\right]^2}. \tag{2.31}$$

Gegenbauer approximation in certain Hilbert spaces and application to singular differential equations are investigated in [31]. Since Jacobi polynomials can be written in terms of hypergeometric functions as in (2.27), and Gegenbauer polynomials are special cases of the Jacobi polynomials, Gegenbauer polynomials can also be written by the hypergeometric function. More specifically, it can be written in a much simpler way, see in ([30], P981), as:

$$C_{2n}^{\lambda}(t) = \frac{(-1)^n}{(\lambda+n)\, B(\lambda, n+1)}\, {}_2F_1\left(-n, n+\lambda; \frac{1}{2}; t^2\right);$$

$$C_{2n+1}^{\lambda}(t) = \frac{(-1)^n\, 2t}{B(\lambda, n+1)}\, {}_2F_1\left(-n, n+\lambda+1; \frac{3}{2}; t^2\right).$$

Using the linear transformation in (2.23), we have

$$C_{2n}^{\lambda}(t) = \frac{(\lambda)_n}{(1)_n} \frac{\left(\lambda+\frac{1}{2}\right)_n}{\left(\frac{1}{2}\right)_n}\, {}_2F_1\left(-n, n+\lambda; \lambda+\frac{1}{2}; 1-t^2\right); \tag{2.32}$$

$$C_{2n+1}^{\lambda}(t) = \frac{2\lambda\,(\lambda+1)_n}{(1)_n} \frac{\left(\lambda+\frac{1}{2}\right)_n}{\left(\frac{3}{2}\right)_n}\, t\, {}_2F_1\left(-n, n+\lambda+1; \lambda+\frac{1}{2}; 1-t^2\right). \tag{2.33}$$

Remark 2.1 *Note that when $\lambda = 0$, coefficient in equation (2.28) makes it unable to represent Chebyshev polynomials. Nevertheless*

$$T_n(t) = \frac{n}{2} \lim_{\lambda \to 0} \left(\frac{C_n^{\lambda}(t)}{\lambda}\right), \ n \geq 1.$$

And we can prove the relation between Chebyshev polynomial and Hypergeometric function as

$$T_{2n}(t) = {}_2F_1\left(-n, n; \frac{1}{2}; 1-t^2\right);$$

$$T_{2n+1}(t) = t\, {}_2F_1\left(-n, n+1; \frac{1}{2}; 1-t^2\right).$$

So in later chapters and sections, we still write $T_n(t) = C_n^0(t)$.

2.7 Modified rational functions

Given $t \in I = [-1, 1]$, $x \in \mathbb{R} = (-\infty, \infty)$, we can use the following algebraic mapping

$$t = \frac{x}{\sqrt{1+x^2}}, \quad x = \frac{t}{\sqrt{1-t^2}}, \tag{2.34}$$

to define the mapped Jacobi functions as

$$j_n^{\alpha,\beta}(x) = J_n^{\alpha,\beta}(t) = J_n^{\alpha,\beta}\left(\frac{x}{\sqrt{1+x^2}}\right), t \in I, x \in \mathbb{R}.$$

Since

$$\frac{dt}{dx} = \left(1+x^2\right)^{-\frac{3}{2}}, \quad \frac{dx}{dt} = \left(1-t^2\right)^{-\frac{3}{2}},$$

this new family of orthogonal functions satisfy

$$\int_{\mathbb{R}} j_n^{\alpha,\beta}(x)\, j_m^{\alpha,\beta}(x)\, \omega_s^{\alpha,\beta}(x)\, dx = \frac{2^{\alpha+\beta+1}\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}{(2n+\alpha+\beta+1)\, n!\Gamma(n+\alpha+\beta+1)}\delta_{nm}.$$

Here

$$\omega_s^{\alpha,\beta}(x) = \omega^{\alpha,\beta}(t)\frac{dt}{dx} = \left(\frac{\sqrt{x^2+1}-x}{\sqrt{x^2+1}}\right)^{\alpha}\left(\frac{\sqrt{x^2+1}+x}{\sqrt{x^2+1}}\right)^{\beta}\frac{1}{\left(1+x^2\right)^{3/2}}.$$

Then as Gegenbauer polynomials generalize Chebyshev polynomials and Legendre polynomials, we define the following modified rational function by multiplying the mapped Gegenbauer polynomials with $\left\{\frac{1}{\left(1+x^2\right)^{\frac{\lambda+1}{2}}}\right\}$, i.e.,

$$R_n^{\lambda}(x) := \frac{1}{\left(1+x^2\right)^{\frac{\lambda+1}{2}}} C_n^{\lambda}\left(\frac{x}{\sqrt{1+x^2}}\right). \tag{2.35}$$

Then due to (2.29), the modified rational functions satisfy the following three-term recurrence relation:

$$\begin{aligned} &R_0^{\lambda}(x) = \frac{1}{\left(1+x^2\right)^{\frac{\lambda+1}{2}}}, R_n^{\lambda}(x) = \frac{2\lambda x}{\left(1+x^2\right)^{1+\frac{\lambda}{2}}}, \\ &nR_n^{\lambda}(x) = \frac{2x}{\sqrt{1+x^2}}(n+\lambda-1)\, R_{n-1}^{\lambda}(x) - (n+2\lambda-2)\, R_{n-2}^{\lambda}(x), n \geq 2. \end{aligned} \tag{2.36}$$

It can be checked that

$$\lim_{x\to\infty}\left(1+x^2\right)^{\frac{\lambda+1}{2}} R_n^{\lambda}(x) = \frac{(2\lambda)_n}{n!}, \quad \lim_{x\to-\infty}\left(1+x^2\right)^{\frac{\lambda+1}{2}} R_n^{\lambda}(x) = (-1)^n\frac{(2\lambda)_n}{n!}.$$

The modified rational functions are eigenfunctions of the following singular Sturm-Liouville problem

$$\left(1+x^2\right)^{\frac{\lambda+1}{2}}\partial_x\left(\left(1+x^2\right)^{-\lambda+1}\partial_x\left(\left(1+x^2\right)^{\frac{\lambda+1}{2}} v(x)\right)\right) + n(n+2\lambda)\, v(x) = 0, x \in (-\infty, \infty).$$

From (2.31), we have $R_n^{\lambda}(x)$ orthogonal with weight function $\omega(x) = 1$, i.e.

$$\int_{-\infty}^{\infty} R_n^{\lambda}(x)\, R_m^{\lambda}(x)\, dx = \gamma_n^{\lambda}\delta_{nm}.$$

Special cases for modified rational functions such as modified Chebyshev function and modified Legendre functions are studied in [34] and [88], respectively. Also from (2.32), and $1-t^2=\frac{1}{1+x^2}$, we have

$$\begin{aligned} R_{2n}^{\lambda}(x) &= \frac{(\lambda)_n}{(1)_n}\frac{\left(\lambda+\frac{1}{2}\right)_n}{\left(\frac{1}{2}\right)_n}\frac{1}{(1+x^2)^{\frac{\lambda+1}{2}}}\,{}_2F_1\left(-n,n+\lambda;\lambda+\frac{1}{2};\frac{1}{1+x^2}\right) \\ &= \frac{(\lambda)_n}{(1)_n}\frac{\left(\lambda+\frac{1}{2}\right)_n}{\left(\frac{1}{2}\right)_n}\sum_{k=0}^{n}\frac{(-n)_k(n+\lambda)_k}{\left(\lambda+\frac{1}{2}\right)_k k!}\frac{1}{(1+x^2)^{k+\frac{\lambda+1}{2}}}. \end{aligned} \tag{2.37}$$

$$\begin{aligned} R_{2n+1}^{\lambda}(x) &= \frac{2\lambda(\lambda+1)_n}{(1)_n}\frac{\left(\lambda+\frac{1}{2}\right)_n}{\left(\frac{3}{2}\right)_n}\frac{1}{(1+x^2)^{\frac{\lambda+1}{2}}}\frac{x}{\sqrt{1+x^2}}\,{}_2F_1\left(-n,n+\lambda+1;\lambda+\frac{1}{2};\frac{1}{1+x^2}\right) \\ &= \frac{2\lambda(\lambda+1)_n}{(1)_n}\frac{\left(\lambda+\frac{1}{2}\right)_n}{\left(\frac{3}{2}\right)_n}\sum_{k=0}^{n}\frac{(-n)_k(n+\lambda+1)_k}{\left(\lambda+\frac{1}{2}\right)_k k!}\frac{x}{\sqrt{1+x^2}}\frac{1}{(1+x^2)^{k+\frac{\lambda+1}{2}}}. \end{aligned} \tag{2.38}$$

Thus we know that $R_{2n}^{\lambda}(x)$ is a finite sum of

$$\frac{1}{(1+x^2)^{k+\frac{\lambda+1}{2}}},\quad \text{where}\quad k=0,1,...,n.$$

And $R_{2n+1}^{\lambda}(x)$ is a finite sum of

$$\frac{x}{\sqrt{1+x^2}}\frac{1}{(1+x^2)^{k+\frac{\lambda+1}{2}}},\quad \text{where}\quad k=0,1,...,n.$$

We will use this in later computation of fractional derivatives for modified rational functions.

2.8 Fractional Sobolev space

Denote by $H^s\left(\mathbb{R}^d\right)$(with $0<s<1$) the fractional Sobolev spaces defined as

$$H^s\left(\mathbb{R}^d\right)=\left\{u\in L^2\left(\mathbb{R}^d\right):\int_{\mathbb{R}^d}\left(1+|\xi|^{2s}\right)|\mathcal{F}u(\xi)|^2d\xi<+\infty\right\},$$

with norm

$$\|u\|_{H^s}=\left(\|u\|^2+|u|_{H^s}^2\right)^{1/2},\quad |u|_{H^s}=\||\xi|_2^{2s}\hat{u}\|.$$

This definition coincides the following definition

$$W^{s,p}\left(\mathbb{R}^d\right)=\left\{u\in L^p\left(\mathbb{R}^d\right):\frac{|u(x)-u(y)|}{|x-y|^{\frac{d}{p}+s}}\in L^p\left(\mathbb{R}^d\times\mathbb{R}^d\right)\right\},$$

with norm

$$\|u\|_{W^{s,p}}=\left(\int_{\mathbb{R}^d}|u|^pdx+\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\frac{|u(x)-u(y)|^p}{|x-y|^{d+sp}}dxdy\right)^{1/p},$$

and seminorm

$$|u|_{W^{s,p}} = \left(\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \frac{|u(x)-u(y)|^p}{|x-y|^{d+sp}} dxdy\right)^{1/p},$$

for p=2. More information about fractional Sobolev spaces can be found in [1, 19, 57] and the references therein.

2.9 Useful lemmas for approximation error

- Hermite Gauss quadrature. Let P_N be the space of polynomials of degree less than or equal to N and denote

$$\hat{P}_N = \left\{u : u = e^{-x^2/2}v, \forall v \in P_N\right\}.$$

The following Gauss quadrature associate with generalized Hermite function is demonstrated in [75]:

Lemma 2.1 *Let $\{x_j\}_{j=0}^N$ be the zeros of $H_{N+1}(x)$, and let $\{\hat{\omega}_j\}_{j=0}^N$ be given by*

$$\hat{\omega}_j = \frac{\sqrt{\pi}}{(N+1)\hat{H}_N^2(x_j)}$$

Then we have

$$\int_{\mathbb{R}} p(x)\,dx = \sum_{j=0}^{N} p(x_j)\hat{\omega}_j, \quad \forall p \in \hat{P}_{2N+1}. \tag{2.39}$$

- Jacobi- and modified rational-Gauss quadrature. The following Jacobi-Gauss quadrature is demonstrated in [74]:

Lemma 2.2 *Let $\{t_j\}_{j=0}^N$ be the zeros of $J_{N+1}^{\alpha,\beta}(t)$, and the weights $\{\rho_j\}_{j=0}^N$ given by*

$$\rho_j = -\frac{2^{\alpha+\beta}(2N+\alpha+\beta+2)\Gamma(N+\alpha+1)\Gamma(N+\beta+1)}{(N+1)!\Gamma(N+\alpha+\beta+2)J_N^{\alpha,\beta}(t_j)\partial_t J_{N+1}^{\alpha,\beta}(t_j)}.$$

Then

$$\int_{-1}^{1} p(t)(1-t)^{\alpha}(1+t)^{\beta}\,dt = \sum_{j=0}^{N} p(t_j)\rho_j,\ \forall p \in P_{2N+1}. \tag{2.40}$$

For Gauss quadrature associated with modified rational functions, let

$$V_N^{\lambda} = \operatorname{span}\left\{R_n^{\lambda}(x) : n = 0, 1, ..., N\right\}.$$

Then by applying the algebraic mapping in (2.34) to the above Jacobi-Gauss quadrature, the modified rational Gauss quadrature can be obtained as follows:

Theorem 2.1

$$\int_{-\infty}^{\infty} u(x)\,dx = \sum_{j=0}^{N} u(x_j)\,\omega_j, \ \ \forall u \in V_{2N+1}^{\lambda}, \tag{2.41}$$

where $\{x_j\}_{j=0}^{N}$ *are the mapped Jacobi-Gauss nodes, i.e.,* $x_j = \frac{t_j}{\sqrt{1-t_j^2}}$*, and the weights* $\omega_j = (1+x^2)^{\lambda+1}\rho_j$*,* $j = 0, 1, ..., N$*. Here* $\{t_j, \rho_j\}_{j=0}^{N}$ *are the associated Gauss points and weights with Gegenbauer polynomials.*

- Hermite interpolation. Now we turn to the interpolation error estimates for Hermite-Gauss quadrature associated with the generalized Hermite function. Denote the interpolant operator $\hat{I}_N^h : C(\mathbb{R}) \to \hat{P}_N$, which interpolates u at $\{x_j\}_{j=0}^{N}$ with the expansion

$$\left(\hat{I}_N^h u\right)(x) = \sum_{n=0}^{N} \hat{u}_n \widehat{H}_n(x).$$

Here the expansion coefficients $\{\hat{u}_n\}_{n=0}^{N}$ can be computed by

$$\hat{u}_n = \frac{1}{\sqrt{\pi}} \sum_{n=0}^{N} u(x_j)\,\widehat{H}_n(x_j)\,\hat{\omega}_j.$$

Introduce the operator $\hat{\partial} = \partial + x$ and define the Sobolev space

$$\hat{B}^m(\mathbb{R}) = \left\{u : \hat{\partial}_x^k u \in L^2(\mathbb{R}), 0 \le k \le m\right\}, \forall m \in \mathbb{N}.$$

equipped with the norm and semi-norm

$$\|u\|_{\hat{B}^m(\mathbb{R})} = \left(\sum_{k=0}^{m} \left\|\hat{\partial}_x^k u\right\|^2\right)^{1/2}, \quad |u|_{\hat{B}^m(\mathbb{R})} = \left\|\hat{\partial}_x^m u\right\|.$$

The following error estimate is derived in [74]

Lemma 2.3 *Let* $\hat{\partial}_x = \partial_x + x$*. For* $u \in C(\mathbb{R})$ *and* $\hat{\partial}_x^m u \in L^2(\mathbb{R})$ *with fixed* $m \ge 1$*, we have*

$$\left\|\hat{\partial}_x^l \left(\hat{I}_N^h u - u\right)\right\| \lesssim N^{\frac{1}{6}+\frac{l-m}{2}} |u|_{\hat{B}^m(\mathbb{R})}, \quad 0 \le l \le m. \tag{2.42}$$

For multidimensional approximations, introduce the operator $\hat{\partial}_{x_j} = \partial_{x_j} + x_j$, and denote $\hat{\partial}_{\mathbf{x}} = \prod_{j=1}^{d} \hat{\partial}_{x_j}$, $\hat{\partial}_{\mathbf{x}}^k = \prod_{j=1}^{d} \hat{\partial}_{x_j}^{k_j}$. Define accordingly the d-dimensional weighted Sobolev spaces

$$\hat{B}^m\left(\mathbb{R}^d\right) = \left\{u : \hat{\partial}_{\mathbf{x}}^{\mathbf{k}} u \in L^2\left(\mathbb{R}^d\right), 0 \le |\mathbf{k}|_1 \le m\right\}, \forall m \in \mathbb{N}.$$

equipped with the norm and semi-norm

$$\|u\|_{\hat{B}^m(\mathbb{R}^d)} = \left(\sum_{0 \le \mathbf{k} \le m} \left\| \hat{\partial}_{\mathbf{x}}^{\mathbf{k}} u \right\|^2 \right)^{1/2}, \quad |u|_{\hat{B}^m(\mathbb{R}^d)} = \left(\sum_{j=1}^{d} \left\| \hat{\partial}_{x_j}^m u \right\| \right)^{1/2}.$$

Similar results for high dimension was proved in [91]. It was further proved in [54] the error estimates between u and $I_N u$ in fractional Hilbert space that

Lemma 2.4 *For any $u \in \hat{B}^m\left(\mathbb{R}^d\right)$ with $m \ge 1$, and if additionally $m \ge d$, we have*

$$\left\| I_N u - u \right\|_{H^s(\mathbb{R}^d)} \lesssim N^{\frac{d}{6} + \frac{s-m}{2}} |u|_{\hat{B}^m(\mathbb{R}^d)}.$$

- Jacobi and modified rational interpolation.

  For Jacobi polynomials on $[-1,1]$, the interpolation operator $I_N^{\alpha,\beta} : C[-1,1] \to P_N$ is defined by

$$I_N^{\alpha,\beta} u \in P_N \text{ such that } I_N^{\alpha,\beta} u(t_j) = u(t_j), j = 0, 1, ..., N.$$

with the expansion

$$I_N^{\alpha,\beta} u(t) = \sum_{n=0}^{N} \tilde{u}_n^{\alpha,\beta} J_n^{\alpha,\beta}(t),$$

where the coefficients $\left\{\tilde{u}_n^{\alpha,\beta}\right\}_{n=0}^{N}$ are determined by the forward discrete Jacobi transform. To measure the approximation error $I_N^{\alpha,\beta} u - u$, the Jacobi-weighted Sobolev space is introduced as:

$$\hat{B}_{\alpha,\beta}^m(I) = \left\{ u : \partial_t^k u \in L^2_{\alpha+k,\beta+k}(I), 0 \le k \le m \right\}, \forall m \in \mathbb{N}.$$

Then we have the following lemma in [74]

Lemma 2.5 *Let $\alpha, \beta > -1$. For any $u \in B_{\alpha,\beta}^m(I)$ with fixed $m \ge 1$, we have that for $0 \le l \le m \le N+1$,*

$$\begin{aligned} &\left\| \partial_t^l \left(I_N^{\alpha,\beta} u - u \right) \right\|_{\omega_{\alpha+l,\beta+l}} \\ &\quad \lesssim c \sqrt{\frac{(N-m+1)!}{N!}} (N+m)^{l-(m+1)/2} \left\| \partial_x^m u \right\|_{\omega_{\alpha+m,\beta+m}}, \quad 0 \le l \le m. \end{aligned}$$

For modified rational functions, we can easily define the interpolation operator as for the Jacobi polynomials

$$I_N^{\lambda} u \in V_N^{\lambda} \text{ such that } I_N^{\lambda} u\left(x_j\right) = u\left(x_j\right), j = 0, 1, ..., N.$$

with the expansion

$$I_N^{\lambda} u\left(x\right) = \sum_{n=0}^{N} \tilde{u}_n^{\lambda} R_n^{\lambda}\left(x\right),$$

where the coefficients

$$\tilde{u}_n^{\lambda} = \frac{1}{\gamma_n^{\lambda}} \sum_{j=0}^{N} u\left(x_j\right) R_n^{\lambda}\left(x_j\right) \omega_j, \; n = 0, 1, ..., N.$$

We can get the approximation error $I_N^{\lambda} u - u$ by imitating the Jacobi polynomials as in [74]. Moreover special cases are obtained for the approximation error in fractional Hilbert space. For example, for modified Legendre rational functions, introduce the space

$$H_C^r\left(\mathbb{R}\right) = \left\{ u | u \text{ is measurable on } \mathbb{R} \text{ and } \left\| u \right\|_{r,C} < \infty \right\},$$

with the norm

$$\left\| u \right\|_{r,C} = \left\| \left(1 + x^2\right)^{\frac{3}{4}} \partial_x \left(\left(1 + x^2\right)^{\frac{3}{4}} u \right) \right\|_{r-1,A},$$

where

$$H_A^r\left(\mathbb{R}\right) = \left\{ u | u \text{ is measurable on } \mathbb{R} \text{ and } \left\| u \right\|_{r,A} < \infty \right\},$$

with the norm

$$\left\| u \right\|_{r,A} = \left(\sum_{k=0}^{r} \left\| \left(1 + x^2\right)^{\frac{r+k}{2}} \partial_x^k u \right\| \right)^{\frac{1}{2}}.$$

Then it was proved in [88] that

Lemma 2.6 *For any* $u \in H_C^r\left(\mathbb{R}\right)$ *and* $0 \le \mu \le 1 \le r$,

$$\left\| I_N^{\frac{1}{2}} u - u \right\|_{\mu} \lesssim c N^{\mu+1-r} \left\| u \right\|_{r,C}.$$

At the same time, error estimates for modified Chebyshev rational function was derived in [34] that first introduce the operator

$$Au\left(x\right) = -\left(x^2 + 1\right)^{\frac{1}{2}} \partial_x \left(\left(x^2 + 1\right) \partial_x \left(\left(x^2 + 1\right)^{\frac{1}{2}} u\left(x\right) \right) \right).$$

Then for any even $r \geq 0$, define the Sobolev space

$$H_{A_q}^r(\mathbb{R}) = \left\{ u | u \text{ is measurable on } \mathbb{R} \text{ and } \left\| u \right\|_{r,A_q} < \infty \right\}$$

where $\|v\|_{r,A_0} = \|A^{\frac{r}{2}} v\|$, and $q \geq 1$,

$$\left\| u \right\|_{r,A_q} = \left\| \left(1+x^2\right) \partial_x \left(\left(1+x^2\right)^{\frac{1}{2}} u \right) \right\|_{r-1,A_{q-1}}.$$

For any real $r > 0$, the Sobolev space $H_{A_q}^r(\mathbb{R})$ and the corresponding norm $\left\| u \right\|_{r,A_q}$ can be defined by space interpolation. The following lemma was derived

Lemma 2.7 *For any $u \in H_{A_1}^r(\mathbb{R})$ and $0 \leq \mu \leq 1 \leq r$,*

$$\left\| I_N^0 u - u \right\|_\mu \lesssim c N^{\mu+1-r} \left\| u \right\|_{r,A_1}.$$

We will later use this lemma for the convergence analysis of our spectral collocation methods.

2.10 Strang's first lemma

For the sake of completeness, here we give a brief introduction of the Strang's first lemma. Let V be a real Hilbert space, equipped with norm $\|\cdot\|_V$. Consider the following problem in weak formulation:

$$\begin{cases} \text{Find } u \in V \text{such that} \\ a(u,v) = \ell(v), \forall\, v \in V. \end{cases} \tag{2.43}$$

Under the assumptions of Lax-Milgram lemma, the above problem admits a unique solution $u \in V$. Then we review the convergence analysis of the numerical approximations to (2.43). Assume that $X_N \subset X$, and

$$\forall\, v \in V, \inf_{v_N \in X_N} \|v - v_N\|_V \to 0 \text{ as } N \to \infty.$$

Then we consider the following approximation to (2.43) as

$$\begin{cases} \text{Find } u \in V_N \text{ such that} \\ a_N(u,v) = \ell_N(v), \forall\, v \in V_N, \end{cases} \tag{2.44}$$

where $a_N(\cdot,\cdot)$ and $\ell_N(\cdot)$ are suitable approximations to $a(\cdot,\cdot)$ and $\ell(\cdot)$, respectively. Then the following strang's first lemma is derived.

Lemma 2.8 *Assume that the bilinear form $a_N(\cdot,\cdot)$ is uniformly V_N-elliptic, i.e. there exits a constant $\hat{\alpha} > 0$ independent of N such that*

$$a_N(v_N, v_N) \geq \hat{\alpha}\|v_N\|_V^2, \forall v_N \in V_N.$$

and denote by $u \in V$ and $u_N \in V_N$, the unique solutions of (2.43) *and* (2.44)*, respectively. Then there exits a constant $C > 0$ such that*

$$\begin{aligned}\|u - u_N\|_V \leq C\Bigg\{ &\inf_{v_N \in V_N}\left(\|u - v_N\|_V + \sup_{\omega_N \in V_N}\frac{|a(v_N, \omega_N) - a_N(v_N, \omega_N)|}{\|\omega_N\|_V}\right) \\ &+ \sup_{\omega_N \in V_N}\frac{|\ell(\omega_N) - \ell_N(\omega_N)|}{\|\omega_N\|_V}\Bigg\}.\end{aligned} \tag{2.45}$$

Chapter 3

Hermite spectral collocation methods

Spectral methods for unbounded domain has been extensively studied in [74, 75], and also in a review article by Shen and Wang in [73]. Orthogonal polynomials/functions on unbounded intervals are most prominently Laguerre and Hermite polynomials/functions and mapped Jacobi polynomials. For problems in the whole unbounded domain, Hermite polynomials/functions are a natural choice. In this chapter, we propose the spectral collocation methods based on Hermite functions of two forms: over-scaled Hermite function $\{\widetilde{H}_n(x)\}_n$ defined in (2.10) in the first place and then the generalized Hermite function $\{\widehat{H}_n(x)\}_n$ defined in (2.9). We derive the corresponding differentiation matrix with fractional Laplace operator in one and two dimensions. Use of scaling parameter and application to multi-term fractional differential equations are presented. Convergence analysis and numerical examples are also included demonstrating the effectiveness of our method.

3.1 Over-scaled Hermite function $\{\widetilde{H}_n(x)\}_n$

In this section, we consider the spectral collocation method based on the over-scaled Hermite function $\{\widetilde{H}_n(x)\}_n$. First of all, we give a brief procedure of how spectral collocation method is conducted. We assume that the solution of the differential equation admits an exponential decay in infinity, and approximate $u(x)$ with a finite sum of the the basis $\{\widetilde{H}_n(x)\}_n$, i.e.,

$$u(x) \approx u_N(x) = \sum_{n=0}^{N-1} c_n \widetilde{H}_n(x). \tag{3.1}$$

Then we insert the above finite expansion into the fractional PDE in (1.3), and obtain

$$(-\Delta)^{\alpha/2} u_N(x) + \rho u_N(x) = f(x). \tag{3.2}$$

Let $\{x_i\}_{i=0}^{N-1}$ be the roots of the N-th order Hermite polynomials, we then impose the collocation conditions on these collocation points, which leads to the following linear equations

$$\sum_{n=0}^{N-1} c_n (-\Delta)^{\alpha/2} \widetilde{H}_n(x_i) + \rho \sum_{n=0}^{N-1} c_n \widetilde{H}_n(x_i) = f(x_i), \quad i = 0, 1, ..., N-1.$$

Then we can write the above equations into the following linear system

$$\widetilde{\mathcal{D}}^{\alpha} \mathbf{c} + \rho \widetilde{\mathcal{H}} \mathbf{c} = \mathbf{f},$$

where $\mathbf{c} = (c_0, ..., c_{N-1})^T$ is the unknown expansion coefficient vector, and $\widetilde{\mathcal{D}}^{\alpha} \in \mathbb{R}^{N \times N}$ is the differential matrix for fractional Laplace operator with components

$$\widetilde{\mathcal{D}}^{\alpha}_{i,j} = (-\Delta)^{\alpha/2} \widetilde{H}_j(x_i), \quad i, j = 0, 1, ..., N-1.$$

By solving the above linear system one gets the expansion coefficient vector $\mathbf{c}$ and then an approximated solution $u_N(x)$. Next, we shall derive explicit formulas for the components of the differential matrix.

3.1.1 1D case

In this subsection, we present our spectral collocation method with over-scaled Hermite function $\widetilde{H}_n(x)$ in one dimension, i.e., the whole line. First, the fractional Laplacian for $\widetilde{H}_n(x)$ are computed using the even/odd property of Hermite polynomials and represented by confluent hypergeometric. We consider the even terms in the first place. Precisely, we have the following theorem

Theorem 3.1 *For $0 < \alpha < 2$, we have*

$$(-\Delta)^{\alpha/2} \widetilde{H}_{2n}(x) = 2^{\alpha} \frac{(-1)^n \sqrt{(2n)!}}{2^n n!} \frac{\Gamma\left(n + \frac{\alpha}{2} + \frac{1}{2}\right)}{\Gamma\left(n + \frac{1}{2}\right)} {}_1F_1\left(n + \frac{\alpha}{2} + \frac{1}{2}; \frac{1}{2}; -x^2\right).$$

We give here two methods of proof using different definitions of fractional Laplacian.

Method 1 of Proof by definition of fractional Laplacian via (1.5)**.**

Proof. We use here the definition of fractional Laplacian by Fourier transform. First consider the forward Fourier transform of the over-scaled Hermite function $\widetilde{H}_n(x)$, we have

$$\begin{aligned}
\mathcal{F}\Big[\widetilde{H}_{2n}\Big](\xi) &= \frac{1}{\sqrt{2\pi}\sqrt{2^{2n}(2n)!}}\int_{\mathbb{R}} \exp(-x^2)H_{2n}(x)e^{-\mathrm{i}x\xi}dx \\
&= \frac{2}{\sqrt{2\pi}\sqrt{2^{2n}(2n)!}}\int_{\mathbb{R}+} \exp(-x^2)H_{2n}(x)\cos(x\xi)dx \\
&= \frac{(-1)^n}{\sqrt{2}\sqrt{2^{2n}(2n)!}}\xi^{2n}e^{-\frac{\xi^2}{4}}.
\end{aligned}$$

Then by considering the inverse Fourier transform we have

$$\begin{aligned}
(-\Delta)^{\alpha/2}\widetilde{H}_{2n}(x) &= \frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}} |\xi|^{\alpha}\mathcal{F}\Big[\widetilde{H}_{2n}\Big](\xi)e^{\mathrm{i}x\xi}d\xi \\
&= \frac{1}{\sqrt{2\pi}}\frac{(-1)^n}{\sqrt{2}\sqrt{2^{2n}(2n)!}}\int_{\mathbb{R}} |\xi|^{\alpha}\xi^{2n}e^{-\frac{\xi^2}{4}}e^{\mathrm{i}x\xi}d\xi \\
&= \frac{2}{2\sqrt{\pi}}\frac{(-1)^n}{\sqrt{2^{2n}(2n)!}}\int_{\mathbb{R}^+} \xi^{2n+\alpha}e^{-\frac{\xi^2}{4}}\cos(x\xi)d\xi \\
&= \frac{(-1)^n}{\sqrt{\pi}\sqrt{2^{2n}(2n)!}}2^{2n+\alpha}\Gamma\left(\frac{2n+\alpha+1}{2}\right){}_1F_1\left(\frac{2n+\alpha+1}{2};\frac{1}{2};-x^2\right) \\
&= 2^{\alpha}\frac{(-1)^n\sqrt{(2n)!}}{2^n n!}\frac{\Gamma\left(n+\frac{\alpha}{2}+\frac{1}{2}\right)}{\Gamma\left(n+\frac{1}{2}\right)}{}_1F_1\left(n+\frac{\alpha}{2}+\frac{1}{2};\frac{1}{2};-x^2\right).
\end{aligned}$$

This completes the proof. ◻

Method 2 of Proof by definition of fractional Laplacian via (1.4)**.**

Proof. We use the singular representation of fractional Laplacian. First we omit the coefficients in the relation of over-scaled Hermite function $\widetilde{H}_n(x)$ and confluent hypergeometric, and by using (2.3), define

$$h_{2n}(x) = e^{-x^2}{}_1F_1\left(-n;\frac{1}{2};x^2\right) = {}_1F_1\left(n+\frac{1}{2};\frac{1}{2};-x^2\right).$$

Then we compute the fractional Laplacian of $h_{2n}(x)$. By the definition of the fractional Laplacian operator in (1.6) and the definition of confluent hypergeometric function in (2.2), we have

$$
\begin{aligned}
&(-\Delta)^{\alpha/2} h_{2n}(x) \\
=&C_{1,\alpha}\int_0^\infty \frac{2{}_1F_1\big(n+\frac{1}{2};\frac{1}{2};-x^2\big)-{}_1F_1\big(n+\frac{1}{2};\frac{1}{2};-(x-t)^2\big)-{}_1F_1\big(n+\frac{1}{2};\frac{1}{2};-(x+t)^2\big)}{t^{1+\alpha}}dt \\
=&\frac{\Gamma\left(\frac{1}{2}\right)C_{1,\alpha}}{\Gamma\left(n+\frac{1}{2}\right)\Gamma(-n)}\int_0^\infty \frac{\int_0^1 y^{n-\frac{1}{2}}(1-y)^{-n-1}\left(2e^{-x^2y}-e^{-(x-t)^2y}-e^{-(x+t)^2y}\right)dy}{t^{1+\alpha}}dt \\
=&\frac{\Gamma\left(\frac{1}{2}\right)C_{1,\alpha}}{\Gamma\left(n+\frac{1}{2}\right)\Gamma(-n)}\int_0^\infty \frac{\int_0^1 y^{n-\frac{1}{2}}(1-y)^{-n-1}e^{-x^2y}\left(2-e^{-yt^2+2xyt}-e^{-yt^2-2xyt}\right)dy}{t^{1+\alpha}}dt \\
=&\frac{\Gamma\left(\frac{1}{2}\right)C_{1,\alpha}}{\Gamma\left(n+\frac{1}{2}\right)\Gamma(-n)}\int_0^1 y^{n-\frac{1}{2}}(1-y)^{-n-1}dy\,\underbrace{e^{-x^2y}\int_0^\infty \frac{2-e^{-yt^2+2xyt}-e^{-yt^2-2xyt}}{t^{1+\alpha}}dt}_{(I)}.
\end{aligned}
$$

Through integration by part, we also have

$$
\begin{aligned}
e^{x^2y}(I) &= -\frac{1}{\alpha}\int_0^\infty \left(2-e^{-yt^2+2xyt}-e^{-yt^2-2xyt}\right)dt^{-\alpha} \\
&= -\frac{1}{\alpha}\left(2-e^{-yt^2+2xyt}-e^{-yt^2+2xyt}\right)t^{-\alpha}\Big|_0^\infty \\
&\quad +\frac{1}{\alpha}\int_0^\infty t^{-\alpha}\left\{(2yt-2xy)e^{-yt^2+2xyt}+(2yt+2xy)e^{-yt^2-2xyt}\right\}dt \\
&= \frac{2y}{\alpha}\left\{\int_0^\infty t^{-\alpha+1}\left(e^{-yt^2+2xyt}+e^{-yt^2-2xyt}\right)dt\right. \\
&\quad \left. +x\int_0^\infty t^{-\alpha}\left(-e^{-yt^2+2xyt}+e^{-yt^2-2xyt}\right)dt\right\}.
\end{aligned}
$$

Combining (2.3) and (2.6), we obtain

$$
\begin{aligned}
&e^{-x^2y}\int_0^\infty t^{\nu-1}e^{-yt^2+2xyt}dt \\
=&\frac{\Gamma(\nu)}{2^\nu}\left\{y^{-\frac{\nu}{2}}\frac{\Gamma\left(\frac{1}{2}\right)}{\Gamma\left(\frac{1+\nu}{2}\right)}{}_1F_1\left(\frac{1-\nu}{2};\frac{1}{2};-x^2y\right)-y^{\frac{1-\nu}{2}}x\frac{\Gamma\left(-\frac{1}{2}\right)}{\Gamma\left(\frac{\nu}{2}\right)}{}_1F_1\left(\frac{2-\nu}{2};\frac{3}{2};-x^2y\right)\right\}; \quad (3.3)
\end{aligned}
$$

and

$$
\begin{aligned}
&e^{-x^2y}\int_0^\infty t^{\nu-1}e^{-yt^2-2xyt}dt \\
=&\frac{\Gamma(\nu)}{2^\nu}\left\{y^{-\frac{\nu}{2}}\frac{\Gamma\left(\frac{1}{2}\right)}{\Gamma\left(\frac{1+\nu}{2}\right)}{}_1F_1\left(\frac{1-\nu}{2};\frac{1}{2};-x^2y\right)+y^{\frac{1-\nu}{2}}x\frac{\Gamma\left(-\frac{1}{2}\right)}{\Gamma\left(\frac{\nu}{2}\right)}{}_1F_1\left(\frac{2-\nu}{2};\frac{3}{2};-x^2y\right)\right\}. \quad (3.4)
\end{aligned}
$$

Then using together (3.3), (3.4) and properties of Gamma function we get

$$\begin{aligned}
(I) &= \frac{2^{\alpha}}{\alpha} y^{\frac{\alpha}{2}} \frac{\Gamma(2-\alpha)\Gamma\left(\frac{1}{2}\right)}{\Gamma\left(\frac{3-\alpha}{2}\right)} {}_1F_1\left(\frac{\alpha-1}{2}; \frac{1}{2}; -x^2 y\right) \\
&\quad + \frac{2^{\alpha+1}}{\alpha} y^{\frac{\alpha}{2}+1} x^2 \frac{\Gamma(1-\alpha)\Gamma\left(-\frac{1}{2}\right)}{\Gamma\left(\frac{1-\alpha}{2}\right)} {}_1F_1\left(\frac{1+\alpha}{2}; \frac{3}{2}; -x^2 y\right) \\
&= \frac{2\Gamma\left(\frac{2-\alpha}{2}\right)}{\alpha} \left\{ y^{\frac{\alpha}{2}} {}_1F_1\left(\frac{\alpha-1}{2}; \frac{1}{2}; -x^2 y\right) - 2x^2 y^{\frac{\alpha}{2}+1} {}_1F_1\left(\frac{1+\alpha}{2}; \frac{3}{2}; -x^2 y\right) \right\}.
\end{aligned}$$

Thus we have

$$(-\Delta)^{\alpha/2} h_{2n}(x) = \frac{2\Gamma\left(\frac{1}{2}\right)\Gamma\left(\frac{2-\alpha}{2}\right) C_{1,\alpha}}{\alpha\Gamma\left(n+\frac{1}{2}\right)\Gamma(-n)} \{(II) + (III)\},$$

where

$$\begin{aligned}
(II) &= \int_0^1 y^{n+\frac{\alpha}{2}-\frac{1}{2}} (1-y)^{-n-1} {}_1F_1\left(\frac{\alpha-1}{2}; \frac{1}{2}; -x^2 y\right) dy, \\
(III) &= -2x^2 \int_0^1 y^{n+\frac{\alpha}{2}+\frac{1}{2}} (1-y)^{-n-1} {}_1F_1\left(\frac{1+\alpha}{2}; \frac{3}{2}; -x^2 y\right) dy.
\end{aligned}$$

Then by the definition of ${}_1F_1$ (2.1), we have

$$\begin{aligned}
(II) &= \sum_{k=0}^{\infty} \frac{\left(\frac{\alpha-1}{2}\right)_k}{\left(\frac{1}{2}\right)_k} \int_0^1 y^{n+k+\frac{\alpha}{2}-\frac{1}{2}} (1-y)^{-n-1} dy \frac{(-x^2)^k}{k!} \\
&= \sum_{k=0}^{\infty} \frac{\left(\frac{\alpha-1}{2}\right)_k}{\left(\frac{1}{2}\right)_k} \frac{\Gamma\left(n+k+\frac{\alpha}{2}+\frac{1}{2}\right)\Gamma(-n)}{\Gamma\left(k+\frac{\alpha}{2}+\frac{1}{2}\right)} \frac{(-x^2)^k}{k!}.
\end{aligned}$$

and

$$\begin{aligned}
(III) &= -2x^2 \sum_{k=0}^{\infty} \frac{\left(\frac{\alpha+1}{2}\right)_k}{\left(\frac{3}{2}\right)_k} \int_0^1 y^{n+k+\frac{\alpha}{2}+\frac{1}{2}} (1-y)^{-n-1} dy \frac{(-x^2)^k}{k!} \\
&= -2x^2 \sum_{k=0}^{\infty} \frac{\left(\frac{\alpha+1}{2}\right)_k}{\left(\frac{3}{2}\right)_k} \frac{\Gamma\left(n+k+\frac{\alpha}{2}+\frac{3}{2}\right)\Gamma(-n)}{\Gamma\left(k+\frac{\alpha}{2}+\frac{3}{2}\right)} \frac{(-x^2)^k}{k!} \\
&= \sum_{k=0}^{\infty} \frac{\left(\frac{\alpha+1}{2}\right)_k}{\left(\frac{1}{2}\right)_{k+1}} \frac{\Gamma\left(n+k+\frac{\alpha}{2}+\frac{3}{2}\right)\Gamma(-n)}{\Gamma\left(k+\frac{\alpha}{2}+\frac{3}{2}\right)} \frac{(-x^2)^{k+1}}{k!} \\
&= \sum_{k=1}^{\infty} \frac{k\left(\frac{\alpha+1}{2}\right)_{k-1}}{\left(\frac{1}{2}\right)_k} \frac{\Gamma\left(n+k+\frac{\alpha}{2}+\frac{1}{2}\right)\Gamma(-n)}{\Gamma\left(k+\frac{\alpha}{2}+\frac{1}{2}\right)} \frac{(-x^2)^k}{k!}.
\end{aligned}$$

Add together the two equations above, we obtain

$$\begin{aligned}
(II)+(III) &= \sum_{k=0}^{\infty} \frac{\left(\frac{\alpha+1}{2}\right)_k}{\left(\frac{1}{2}\right)_k} \frac{\Gamma\left(n+k+\frac{\alpha}{2}+\frac{1}{2}\right)\Gamma(-n)}{\Gamma\left(k+\frac{\alpha}{2}+\frac{1}{2}\right)} \frac{(-x^2)^k}{k!} \\
&= \frac{\Gamma\left(n+\frac{\alpha}{2}+\frac{1}{2}\right)\Gamma(-n)}{\Gamma\left(\frac{\alpha}{2}+\frac{1}{2}\right)} \sum_{k=0}^{\infty} \frac{\left(n+\frac{\alpha}{2}+\frac{1}{2}\right)_k}{\left(\frac{1}{2}\right)_k} \frac{(-x^2)^k}{k!}.
\end{aligned}$$

Finally, we obtain

$$
\begin{aligned}
(-\Delta)^{\alpha/2} h_{2n}(x) &= 2C_{1,\alpha} \frac{\Gamma\left(\frac{1}{2}\right)\Gamma\left(\frac{2-\alpha}{2}\right)\Gamma\left(n+\frac{\alpha}{2}+\frac{1}{2}\right)}{\alpha\Gamma\left(n+\frac{1}{2}\right)\Gamma\left(\frac{\alpha}{2}+\frac{1}{2}\right)} {}_1F_1\left(n+\frac{\alpha}{2}+\frac{1}{2};\frac{1}{2};-x^2\right) \\
&= 2^{\alpha}\frac{\Gamma\left(n+\frac{\alpha}{2}+\frac{1}{2}\right)}{\Gamma\left(n+\frac{1}{2}\right)} e^{-x^2} {}_1F_1\left(-n-\frac{\alpha}{2};\frac{1}{2};x^2\right). \qquad (3.5)
\end{aligned}
$$

Notice that the above equations valid for $0<\alpha<1$ since (3.3)-(3.4) only holds with $0<\nu<1$. Nevertheless, for any $\alpha\in(0,2)$, we can find $\alpha_1,\alpha_2\in(0,1)$ such that $\alpha=\alpha_1+\alpha_2$, then we have for any $0<\alpha<2$

$$
\begin{aligned}
(-\Delta)^{\alpha/2} h_{2n}(x) &= (-\Delta)^{\alpha_2/2}\left\{(-\Delta)^{\alpha_1/2} h_{2n}(x)\right\} \\
&= 2^{\alpha_1}\frac{\Gamma\left(n+\frac{\alpha_1}{2}+\frac{1}{2}\right)}{\Gamma\left(n+\frac{1}{2}\right)}(-\Delta)^{\alpha_2/2}\left\{e^{-x^2} {}_1F_1\left(-n-\frac{\alpha_1}{2};\frac{1}{2};x^2\right)\right\} \\
&= 2^{\alpha_1+\alpha_2}\frac{\Gamma\left(n+\frac{\alpha_1}{2}+\frac{\alpha_2}{2}+\frac{1}{2}\right)}{\Gamma\left(n+\frac{1}{2}\right)} e^{-x^2} {}_1F_1\left(-n-\frac{\alpha_1}{2}-\frac{\alpha_2}{2};\frac{1}{2};x^2\right) \\
&= 2^{\alpha}\frac{\Gamma\left(n+\frac{\alpha}{2}+\frac{1}{2}\right)}{\Gamma\left(n+\frac{1}{2}\right)} e^{-x^2} {}_1F_1\left(-n-\frac{\alpha}{2};\frac{1}{2};x^2\right).
\end{aligned}
$$

Consequently, (3.5) holds for all $0<\alpha<2$ and the proof is complete by noticing the relationship between $h_{2n}(x)$ and $\widetilde{H}_{2n}(x)$ that

$$
\widetilde{H}_{2n}(x) = (-1)^n\frac{(2n)!}{n!}\frac{1}{\sqrt{2^{2n}(2n)!}} h_{2n}(x).
$$

$\square$

In the above derivation, we have adopted some integral formulas in [36]. Using similar arguments, for the odd terms $\widetilde{H}_{2n+1}(x)$, we have the following theorem

Theorem 3.2 *For $0<\alpha<2$, it holds*

$$
\begin{aligned}
& (-\Delta)^{\alpha/2}\widetilde{H}_{2n+1}(x) \\
= \; & 2^{\alpha+1}\frac{(-1)^n\sqrt{(2n+1)!}}{2^{n+\frac{1}{2}}n!}\frac{\Gamma\left(n+\frac{\alpha}{2}+\frac{3}{2}\right)}{\Gamma\left(n+\frac{3}{2}\right)} x\,{}_1F_1\left(n+\frac{\alpha}{2}+\frac{3}{2};\frac{3}{2};-x^2\right). \qquad (3.6)
\end{aligned}
$$

We also give here two methods of proof using different definitions of fractional Laplacian.

Method 1 of Proof by definition of fractional Laplacian via (1.5)**.**

Proof. Consider the forward Fourier transform, we have

$$\begin{aligned}
\mathcal{F}\left[\widetilde{H}_{2n+1}\right](\xi) &= \frac{1}{\sqrt{2\pi}\sqrt{2^{2n+1}(2n+1)!}}\int_{\mathbb{R}} \exp(-x^2)H_{2n+1}(x)e^{-\mathrm{i}x\xi}dx \\
&= \frac{-2i}{\sqrt{2\pi}\sqrt{2^{2n+1}(2n+1)!}}\int_{\mathbb{R}+} \exp(-x^2)H_{2n+1}(x)\sin(x\xi)dx \\
&= \frac{(-1)^{n+1}i}{\sqrt{2}\sqrt{2^{2n+1}(2n+1)!}}\xi^{2n+1}e^{-\frac{\xi^2}{4}}.
\end{aligned}$$

Then by considering the inverse Fourier transform we have

$$\begin{aligned}
(-\Delta)^{\alpha/2}\widetilde{H}_{2n+1}(x) &= \frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}}|\xi|^{\alpha}\mathcal{F}\left[\widetilde{H}_{2n+1}\right](\xi)e^{\mathrm{i}x\xi}d\xi \\
&= \frac{1}{\sqrt{2\pi}}\frac{(-1)^{n+1}i}{\sqrt{2}\sqrt{2^{2n+1}(2n+1)!}}\int_{\mathbb{R}}|\xi|^{\alpha}\xi^{2n+1}e^{-\frac{\xi^2}{4}}e^{\mathrm{i}x\xi}d\xi \\
&= \frac{1}{\sqrt{\pi}}\frac{(-1)^{n}}{\sqrt{2^{2n+1}(2n+1)!}}\int_{\mathbb{R}+}\xi^{2n+\alpha+1}e^{-\frac{\xi^2}{4}}\sin(x\xi)d\xi \\
&= \frac{(-1)^n 2^{2n+\alpha+2}\Gamma\left(\frac{2n+\alpha+3}{2}\right)}{\sqrt{\pi}\sqrt{2^{2n+1}(2n+1)!}}x{}_1F_1\left(\frac{2n+\alpha+3}{2};\frac{3}{2};-x^2\right) \\
&= 2^{\alpha+1}\frac{(-1)^n\sqrt{(2n+1)!}}{2^{n+\frac{1}{2}}n!}\frac{\Gamma\left(n+\frac{\alpha}{2}+\frac{3}{2}\right)}{\Gamma\left(n+\frac{3}{2}\right)}x{}_1F_1\left(n+\frac{\alpha}{2}+\frac{3}{2};\frac{3}{2};-x^2\right).
\end{aligned}$$

This completes the proof. $\square$

Method 2 of Proof by definition of fractional Laplacian via (1.4).

Proof. Let

$$h_{2n+1}(x) = xe^{-x^2}{}_1F_1\left(-n;\frac{3}{2};x^2\right) = {}_1F_1\left(n+\frac{3}{2};\frac{3}{2};-x^2\right).$$

By the definition of the fractional Laplacian operator, we have

$$\begin{aligned}
&(-\Delta)^{\alpha/2}h_{2n+1}(x) \\
=& C_{1,\alpha}\int_0^{\infty}\frac{2x{}_1F_1\left(n+\frac{3}{2};\frac{3}{2};-x^2\right)-(x-t){}_1F_1\left(n+\frac{3}{2};\frac{3}{2};-(x-t)^2\right)-(x+t){}_1F_1\left(n+\frac{3}{2};\frac{3}{2};-(x+t)^2\right)}{t^{1+\alpha}}dt \\
=& \frac{\Gamma(\frac{3}{2})C_{1,\alpha}}{\Gamma(n+\frac{3}{2})\Gamma(-n)}\int_0^{\infty}\frac{\int_0^1 y^{n+\frac{1}{2}}(1-y)^{-n-1}\left(2xe^{-x^2y}-(x-t)e^{-(x-t)^2y}-(x+t)e^{-(x+t)^2y}\right)dy}{t^{1+\alpha}}dt \\
=& \frac{\Gamma(\frac{3}{2})C_{1,\alpha}}{\Gamma(n+\frac{3}{2})\Gamma(-n)}\int_0^{\infty}\frac{\int_0^1 y^{n+\frac{1}{2}}(1-y)^{-n-1}e^{-x^2y}\left(2x-(x-t)e^{-yt^2+2xyt}-(x+t)e^{-yt^2-2xyt}\right)dy}{t^{1+\alpha}}dt \\
=& \frac{\Gamma(\frac{3}{2})C_{1,\alpha}}{\Gamma(n+\frac{3}{2})\Gamma(-n)}\int_0^1 y^{n+\frac{1}{2}}(1-y)^{-n-1}dy\,\underbrace{e^{-x^2y}\int_0^{\infty}\frac{2x-(x-t)e^{-yt^2+2xyt}-(x+t)e^{-yt^2-2xyt}}{t^{1+\alpha}}dt}_{(IV)}.
\end{aligned}$$

Then we divide (IV) into two parts:

$$(IV) = x\int_0^{\infty}\frac{2-e^{-yt^2+2xyt}-e^{-yt^2-2xyt}}{t^{1+\alpha}}dt+\int_0^{\infty}t^{-\alpha}\left(e^{-yt^2+2xyt}-e^{-yt^2-2xyt}\right)dt.$$

Similar to the case for even terms when we compute (I), we have

$$(IV) = x\frac{2\Gamma(\frac{2-\alpha}{2})}{\alpha}\left\{y^{\frac{\alpha}{2}}{}_1F_1\left(\frac{\alpha-1}{2};\frac{1}{2};-x^2y\right) - 2x^2y^{\frac{\alpha}{2}+1}{}_1F_1\left(\frac{1+\alpha}{2};\frac{3}{2};-x^2y\right)\right\}$$
$$+ 2x\Gamma(\frac{2-\alpha}{2})y^{\frac{\alpha}{2}}{}_1F_1\left(\frac{1+\alpha}{2};\frac{3}{2};-x^2y\right).$$

Take it back

$$(-\Delta)^{\frac{\alpha}{2}}h_{2n+1}(x) = \frac{2x\Gamma(\frac{3}{2})\Gamma(\frac{2-\alpha}{2})C_{1,\alpha}}{\alpha\Gamma(n+\frac{3}{2})\Gamma(-n)}\left\{\underbrace{\int_0^1 y^{n+\frac{\alpha}{2}+\frac{1}{2}}(1-y)^{-n-1}{}_1F_1\left(\frac{\alpha-1}{2};\frac{1}{2};-x^2y\right)dy}_{(V)}\right.$$
$$\underbrace{+(-2x^2)\int_0^1 y^{n+\frac{\alpha}{2}+\frac{3}{2}}(1-y)^{-n-1}{}_1F_1\left(\frac{\alpha+1}{2};\frac{3}{2};-x^2y\right)dy}_{(VI)}$$
$$\left.\underbrace{+\alpha\int_0^1 y^{n+\frac{\alpha}{2}+\frac{1}{2}}(1-y)^{-n-1}{}_1F_1\left(\frac{\alpha+1}{2};\frac{3}{2};-x^2y\right)dy}_{(VII)}\right\}.$$

Then by the definition of ${}_1F_1$ by power series, we have

$$\begin{aligned}(V) &= \sum_{k=0}^{\infty}\frac{(\frac{\alpha-1}{2})_k}{(\frac{1}{2})_k}\int_0^1 y^{n-\beta+k+\frac{\alpha}{2}+\frac{1}{2}}(1-y)^{-n-1}dy\frac{(-x^2)^k}{k!}\\ &= \sum_{k=0}^{\infty}\frac{(\frac{\alpha-1}{2})_k}{(\frac{1}{2})_k}\frac{\Gamma(n+k+\frac{\alpha}{2}+\frac{3}{2})\Gamma(-n)}{\Gamma(k+\frac{\alpha}{2}+\frac{3}{2})}\frac{(-x^2)^k}{k!}.\end{aligned}$$

and

$$\begin{aligned}(VI) &= (-2x^2)\sum_{k=0}^{\infty}\frac{(\frac{\alpha+1}{2})_k}{(\frac{3}{2})_k}\int_0^1 y^{n+k+\frac{\alpha}{2}+\frac{3}{2}}(1-y)^{-n-1}dy\frac{(-x^2)^k}{k!}\\ &= (-2x^2)\sum_{k=0}^{\infty}\frac{(\frac{\alpha+1}{2})_k}{(\frac{3}{2})_k}\frac{\Gamma(n+k+\frac{\alpha}{2}+\frac{5}{2})\Gamma(-n)}{\Gamma(k+\frac{\alpha}{2}+\frac{5}{2})}\frac{(-x^2)^k}{k!}\\ &= \sum_{k=1}^{\infty}\frac{k(\frac{\alpha+1}{2})_{k-1}}{(\frac{1}{2})_k}\frac{\Gamma(n+k+\frac{\alpha}{2}+\frac{3}{2})\Gamma(-n)}{\Gamma(k+\frac{\alpha}{2}+\frac{3}{2})}\frac{(-x^2)^k}{k!}.\end{aligned}$$

Add these two terms

$$(V)+(VI) = \sum_{k=0}^{\infty}\frac{(\frac{\alpha+1}{2})_k}{(\frac{1}{2})_k}\frac{\Gamma(n+k+\frac{\alpha}{2}+\frac{3}{2})\Gamma(-n)}{\Gamma(k+\frac{\alpha}{2}+\frac{3}{2})}\frac{(-x^2)^k}{k!}.$$

Also we have

$$\begin{aligned}(VII) &= \alpha\sum_{k=0}^{\infty}\frac{(\frac{\alpha+1}{2})_k}{(\frac{3}{2})_k}\int_0^1 y^{n+k+\frac{\alpha}{2}+\frac{1}{2}}(1-y)^{-n-1}dy\frac{(-x^2)^k}{k!}\\ &= \alpha\sum_{k=0}^{\infty}\frac{(\frac{\alpha+1}{2})_k}{(\frac{3}{2})_k}\frac{\Gamma(n+k+\frac{\alpha}{2}+\frac{3}{2})\Gamma(-n)}{\Gamma(k+\frac{\alpha}{2}+\frac{3}{2})}\frac{(-x^2)^k}{k!}.\end{aligned}$$

For any integer k, we have

$$\left(\frac{1}{2}\right)_k = \frac{\frac{1}{2}\left(\frac{3}{2}\right)_k}{\frac{3}{2}+k-1} = \frac{\left(\frac{3}{2}\right)_k}{2\left(\frac{1}{2}+k\right)}.$$

So add (V), (VI) and (VII), we have

$$\begin{aligned}
(V)+(VI)+(VII) &= \sum_{k=0}^{\infty}\left\{\frac{1}{(\frac{1}{2})_k}+\frac{\alpha}{(\frac{3}{2})_k}\right\}\left(\frac{\alpha+1}{2}\right)_k \frac{\Gamma(n+k+\frac{\alpha}{2}+\frac{3}{2})\Gamma(-n)}{\Gamma(k+\frac{\alpha}{2}+\frac{3}{2})}\frac{(-x^2)^k}{k!} \\
&= 2\frac{\alpha+1}{2}\sum_{k=0}^{\infty}\frac{(\frac{\alpha+3}{2})_k}{(\frac{3}{2})_k}\frac{\Gamma(n+k+\frac{\alpha}{2}+\frac{3}{2})\Gamma(-n)}{\Gamma(k+\frac{\alpha}{2}+\frac{3}{2})}\frac{(-x^2)^k}{k!} \\
&= 2\frac{\Gamma(-n)\Gamma(n+\frac{\alpha}{2}+\frac{3}{2})}{\Gamma(\frac{\alpha}{2}+\frac{1}{2})}{}_1F_1(n+\frac{\alpha}{2}+\frac{3}{2};\frac{3}{2};-x^2).
\end{aligned}$$

Finally

$$\begin{aligned}
(-\Delta)^{\frac{\alpha}{2}}h_{2n+1}(x) &= \frac{2xC_{1,\alpha}\Gamma(\frac{3}{2})\Gamma(\frac{2-\alpha}{2})}{\alpha\Gamma(n+\frac{3}{2})\Gamma(-n)}\frac{2\Gamma(-n)\Gamma(n+\frac{\alpha}{2}+\frac{3}{2})}{\Gamma(\frac{\alpha}{2}+\frac{1}{2})}{}_1F_1(n+\frac{\alpha}{2}+\frac{3}{2};\frac{3}{2};-x^2) \\
&= 2xC_{1,\alpha}\frac{\Gamma(\frac{1}{2})\Gamma(\frac{2-\alpha}{2})\Gamma(n+\frac{\alpha}{2}+\frac{3}{2})}{\alpha\Gamma(n+\frac{3}{2})\Gamma(\frac{\alpha}{2}+\frac{1}{2})}{}_1F_1(n+\frac{\alpha}{2}+\frac{3}{2};\frac{3}{2};-x^2) \\
&= 2^{\alpha}\frac{\Gamma(n+\frac{\alpha}{2}+\frac{3}{2})}{\Gamma(n+\frac{3}{2})}xe^{-x^2}{}_1F_1(-n-\frac{\alpha}{2};\frac{3}{2};x^2).
\end{aligned}$$

The proof is complete by noticing the relationship between $h_{2n+1}(x)$ and $\widetilde{H}_{2n+1}(x)$ that

$$\widetilde{H}_{2n+1}(x) = 2(-1)^n\frac{(2n+1)!}{n!}\frac{1}{\sqrt{2^{2n}(2n)!}}h_{2n+1}(x).$$

□

By Theorems 3.1-3.2, we get the following explicit formula for the components of the differential matrix (DM)

$$\begin{aligned}
\widetilde{\mathcal{D}}^{\alpha}_{ij} &= (-\Delta)^{\alpha/2}\widetilde{H}_j(x_i) \\
&= \begin{cases} 2^{\alpha}\dfrac{(-1)^n\sqrt{(2n)!}}{2^n n!}\dfrac{\Gamma\left(n+\frac{\alpha}{2}+\frac{1}{2}\right)}{\Gamma\left(n+\frac{1}{2}\right)}{}_1F_1\left(n+\dfrac{\alpha}{2}+\dfrac{1}{2};\dfrac{1}{2};-x_i^2\right), & j=2n; \\ 2^{\alpha+1}\dfrac{(-1)^n\sqrt{(2n+1)!}}{2^{n+\frac{1}{2}}n!}\dfrac{\Gamma\left(n+\frac{\alpha}{2}+\frac{3}{2}\right)}{\Gamma\left(n+\frac{3}{2}\right)}x_i{}_1F_1\left(n+\dfrac{\alpha}{2}+\dfrac{3}{2};\dfrac{3}{2};-x_i^2\right), & j=2n+1. \end{cases}
\end{aligned} \tag{3.7}$$

We now summarize the procedure for computing the components of the DM:

- For each x_i, compute the quantities $\widetilde{\mathcal{D}}^{\alpha}_{ij}$ with $j=0,1,2,3$, by the above formula. Notice that one has to deal with confluent hypergeometric function ${}_1F_1$ and this may be non-trivial, as by definition (2.1), which is an infinite expansion or in (2.2) as an integral. Nevertheless, one can find a fast & accurate algorithm for example in [62].

- Compute the quantities $\widetilde{\mathcal{D}}_{ij}^{\alpha}$ for $4 < j \leq N-1$ in a recurrence way using the recurrence formula of confluent hypergeometric function in (2.4).

In general, the above DM is easy to construct, and in fact, the matrix can be stored in priori (offline). We provide in Fig. 3.1 the condition number of the differential matrix with respect to the number of collocation points N. It is noticed that the condition number grows very fast with respect to N. Thus, efficient pre-conditioners should be designed for practice applications.

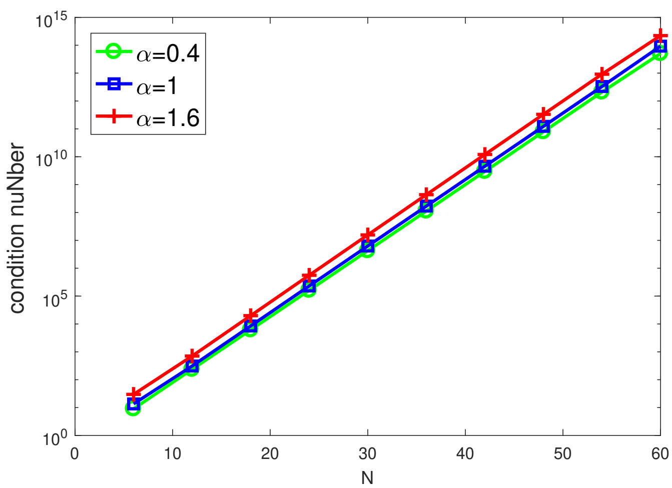

Figure 3.1: Condition number of the differentiation matrix for over-scaled Hermite function $\widetilde{H}_n(x)$ versus N.

3.1.2 2D case

For multi-dimensional cases, the bases used will be the tensorized 1D bases. Here we take the two dimensional case as an example, and generalizations to three dimensional cases may involve complex derivations and we omit it here. To this end, the two dimensional bases take the following form $\{\widetilde{H}_n(x)\widetilde{H}_m(y)\}_{n,m}$.

By (1.5), we know that

$$\begin{aligned}\mathcal{F}\left[\widetilde{H}_n\widetilde{H}_m\right](\xi,\eta) &= \frac{1}{2\pi}\int_{\mathbb{R}}\int_{\mathbb{R}}\widetilde{H}_n(x)\widetilde{H}_m(y)e^{-\mathrm{i}x\xi}e^{-\mathrm{i}y\eta}dxdy \\ &= \frac{1}{2\pi}\int_{\mathbb{R}}\widetilde{H}_n(x)e^{-\mathrm{i}x\xi}dx\int_{\mathbb{R}}\widetilde{H}_m(y)e^{-\mathrm{i}y\eta}dy = \mathcal{F}\left[\widetilde{H}_n\right](\xi)\mathcal{F}\left[\widetilde{H}_m\right](\eta).\end{aligned}$$

Then, using the inverse Fourier transform gives

$$\begin{aligned}
&(-\Delta)^{\alpha/2}\left[\widetilde{H}_n(x)\widetilde{H}_m(y)\right] \\
&= \frac{1}{2\pi}\int_{\mathbb{R}}\int_{\mathbb{R}} \left(\xi^2+\eta^2\right)^{\frac{\alpha}{2}} \mathcal{F}\left[\widetilde{H}_n\right](\xi)\mathcal{F}\left[\widetilde{H}_m\right](\eta) e^{\mathrm{i}x\xi}e^{\mathrm{i}y\eta}d\xi d\eta. \qquad (3.8)
\end{aligned}$$

We take the double-even term $\{\widetilde{H}_{2n}(x)\widetilde{H}_{2m}(y)\}$ as an example, and denote

$$L_{nm} = \frac{(-1)^n}{\sqrt{2}\sqrt{2^{2n}(2n)!}}\frac{(-1)^m}{\sqrt{2}\sqrt{2^{2m}(2m)!}}.$$

Then we have

$$\begin{aligned}
&(-\Delta)^{\alpha/2}\left[\widetilde{H}_{2n}(x)\widetilde{H}_{2m}(y)\right] \\
&= \frac{L_{nm}}{2\pi}\int_{\mathbb{R}}\int_{\mathbb{R}} \left(\xi^2+\eta^2\right)^{\frac{\alpha}{2}} \xi^{2n}e^{-\frac{\xi^2}{4}}\eta^{2m}e^{-\frac{\eta^2}{4}}e^{\mathrm{i}x\xi}e^{\mathrm{i}y\eta}d\xi d\eta \\
&= \frac{4L_{nm}}{2\pi}\int_{\mathbb{R}+}\int_{\mathbb{R}+} \left(\xi^2+\eta^2\right)^{\frac{\alpha}{2}} \xi^{2n}e^{-\frac{\xi^2}{4}}\eta^{2m}e^{-\frac{\eta^2}{4}}\cos(x\xi)\cos(y\eta)d\xi d\eta \\
&= \frac{4L_{nm}}{2\pi}\int_{\mathbb{R}+} \mathcal{I}(x,y,\rho)\ \rho^{2n+2m+\alpha+1}e^{-\frac{\rho^2}{4}}d\rho,
\end{aligned}$$

where

$$\mathcal{I}(x,y,\rho) = \int_0^{\frac{\pi}{2}} (\cos\theta)^{2n}(\sin\theta)^{2m}\cos(x\rho\cos\theta)\cos(y\rho\sin\theta)d\theta.$$

By the definition of the Bessel function (2.12) and the property (2.16) we have

$$\begin{aligned}
&\int_0^{\frac{\pi}{2}} (\cos\theta)^{2n}(\sin\theta)^{2m}\cos(p\cos\theta)\cos(q\sin\theta)d\theta \\
&= \frac{\pi}{2}(pq)^{\frac{1}{2}}\int_0^1 (1-x^2)^{n-\frac{1}{4}}x^{2m+\frac{1}{2}}J_{-\frac{1}{2}}(p\sqrt{1-x^2})J_{-\frac{1}{2}}(qx)dx \\
&= \frac{\pi}{2}\left(\frac{\partial}{p\partial p}\right)^n\left(\frac{\partial}{q\partial q}\right)^m\left[\left(\sqrt{p^2+q^2}\right)^{-(n+m)}J_{n+m}\left(\sqrt{p^2+q^2}\right)\right].
\end{aligned}$$

Notice that by property (2.14) we have

$$\begin{aligned}
&\left(\frac{\partial}{p\partial p}\right)^n\left(\frac{\partial}{q\partial q}\right)^m\left[\left(\sqrt{p^2+q^2}\right)^{-(n+m)}J_{n+m}\left(\sqrt{p^2+q^2}\right)\right] \\
&= (-1)^{n+m}\left(\sqrt{p^2+q^2}\right)^{-(2n+2m)}J_{2n+2m}\left(\sqrt{p^2+q^2}\right).
\end{aligned}$$

Now, by replacing p and q with ρx and ρy, we obtain

$$\mathcal{I}(x,y,\rho) = \frac{\pi}{2}(-1)^{n+m}\rho^{-(2n+2m)}\left(\sqrt{x^2+y^2}\right)^{-(2n+2m)}J_{2n+2m}\left(\rho\sqrt{x^2+y^2}\right).$$

We then do inverse Fourier transform to obtain (for $t = m + n$)

$$
\begin{aligned}
&(-\Delta)^{\alpha/2}\left[\widetilde{H}_{2n}(x)\widetilde{H}_{2m}(y)\right] \\
&= (-1)^t L_{nm}(x^2+y^2)^{-t}\int_{\mathbb{R}^+}\rho^{\alpha+1}e^{-\frac{\rho^2}{4}}J_{2t}\left(\rho\sqrt{x^2+y^2}\right)d\rho \\
&= \frac{2^\alpha\Gamma(t+\frac{\alpha}{2}+1)}{\sqrt{2^{2n}(2n)!}\sqrt{2^{2m}(2m)!}\Gamma(2t+1)}\,{}_1F_1\left(t+\frac{\alpha}{2}+1;2t+1;-\left(x^2+y^2\right)\right).
\end{aligned}
$$

In the above derivation, we have used the property (2.13). In a similar way, we can derive similar results for the bases of forms $\widetilde{H}_{2n+1}(x)\widetilde{H}_{2m}(y)$, $\widetilde{H}_{2n}(x)\widetilde{H}_{2m+1}(y)$ and $\widetilde{H}_{2n+1}(x)\widetilde{H}_{2m+1}(y)$. To summaries these results in an unified way, we introduce the parameter δ_1 and δ_2, with $\delta_1, \delta_2 \in \{0,1\}$. And let

$$
a = n+m+\frac{\alpha}{2}+\delta_1+\delta_2+1; \quad b = 2n+2m+\delta_1+\delta_2+1.
$$

Using similar arguments as above, we can derive that

$$
(-\Delta)^{\alpha/2}\left[\widetilde{H}_{2n+\delta_1}(x)\widetilde{H}_{2m+\delta_2}(y)\right] = C_{x,y}(\alpha,m,n,\delta_1,\delta_2)\frac{\Gamma(a)}{\Gamma(b)}\,{}_1F_1\left(a;b;-\left(x^2+y^2\right)\right),
$$

with

$$
C_{x,y}(\alpha,m,n,\delta_1,\delta_2) = \frac{2^{\alpha+\delta_1+\delta_2}x^{\delta_1}y^{\delta_2}}{\sqrt{2^{2n+\delta_1}(2n+\delta_1)!}\sqrt{2^{2m+\delta_2}(2m+\delta_2)!}}.
$$

We finally provide the explicit formulas for the components of the DM as following

$$
\widetilde{\mathcal{D}}^\alpha_{(i-1)*N+j,(p-1)*N+q} = (-\Delta)^{\alpha/2}\left\{\widetilde{H}_p(x_i)\widetilde{H}_q(y_j)\right\} \tag{3.9}
$$

$$
= \begin{cases}
\dfrac{2^\alpha\Gamma(n+m+\frac{\alpha}{2}+1)\,{}_1F_1\left(n+m+\frac{\alpha}{2}+1;2n+2m+1;-\left(x_i^2+y_j^2\right)\right)}{\sqrt{2^{2n}(2n)!}\sqrt{2^{2m}(2m)!}\Gamma(2n+2m+1)}, \\
\qquad\qquad p=2n, q=2m; \\
\dfrac{2^{\alpha+1}\Gamma(n+m+\frac{\alpha}{2}+2)y_j\,{}_1F_1\left(n+m+\frac{\alpha}{2}+2;2n+2m+2;-\left(x_i^2+y_j^2\right)\right)}{\sqrt{2^{2n}(2n)!}\sqrt{2^{2m+1}(2m+1)!}\Gamma(2n+2m+2)}, \\
\qquad\qquad p=2n, q=2m+1; \\
\dfrac{2^{\alpha+1}\Gamma(n+m+\frac{\alpha}{2}+2)x_i\,{}_1F_1\left(n+m+\frac{\alpha}{2}+2;2n+2m+2;-\left(x_i^2+y_j^2\right)\right)}{\sqrt{2^{2n+1}(2n+1)!}\sqrt{2^{2m}(2m)!}\Gamma(2n+2m+2)}, \\
\qquad\qquad p=2n+1, q=2m; \\
\dfrac{2^{\alpha+2}\Gamma(n+m+\frac{\alpha}{2}+3)x_iy_j\,{}_1F_1\left(n+m+\frac{\alpha}{2}+3;2n+2m+3;-\left(x_i^2+y_j^2\right)\right)}{\sqrt{2^{2n+1}(2n+1)!}\sqrt{2^{2m+1}(2m+1)!}\Gamma(2n+2m+3)}, \\
\qquad\qquad p=2n+1, q=2m+1.
\end{cases}
$$

Again, the above components can be computed in a similar procedure as in the one-dimensional case. We remark that one may also derive such formulas for the three dimensional case, and we omit this here as it may involves complex notations.

3.1.3 The use of the scaling factors

It is well known that for Hermite-type spectral methods, the convergence rate deteriorates if the decay rates between the solution and the basis function have a relatively large gap. A remedy to fix this problem is to use the so-called scaling factor [53, 79]. We now introduce the basic idea of the scaling factor and choose the one-dimensional case as an example for illustration. To this end, let $u(x)$ be a function that decay exponentially, namely,

$$|u(x)| \sim 0, \quad \forall\, |x| > M, \tag{3.10}$$

where $M > 0$ is some constant. The idea of using the scaling factor is to expand u as

$$u(x) = \sum_{n=0}^{N-1} c_n \widetilde{H}_n(rx) \;\Leftrightarrow\; u\left(x/r\right) = \sum_{n=0}^{N-1} c_n \widetilde{H}_n(x), \tag{3.11}$$

where $r > 0$ is a scaling factor. The key point of using r is to scale the Hermite-Gauss nodes $\{x_k\}_{k=0}^{N-1}$ so that the collocation points $\{x_k/r\}_{k=0}^{N-1}$ are well within the effective support of u. This suggests the following choice

$$\max_{0\le k\le N-1} \{|x_k|\}/r \le M \quad \Rightarrow \quad r = \max_{0\le k\le N-1} \{|x_k|\}/M. \tag{3.12}$$

We remark however, in practice, finding the quantity M may be non-trivial and thus the optimal scaling factor is hard to obtain in general.

We now show how to include the scaling factor in our spectral collocation methods for the fractional PDEs. Let us illustrate the idea in 1D. We now seek to the following expansion

$$u_N(x) = \sum_{n=0}^{N-1} c_n \widetilde{H}_n(rx).$$

By inserting the expansion to the fractional PDE (1.3) and imposing the collocation condition we obtain

$$\widetilde{\mathcal{D}}^{\alpha,r}\mathbf{c} + \rho\widetilde{\mathcal{H}}^{r}\mathbf{c} = \mathbf{f}, \tag{3.13}$$

where the $\widetilde{\mathcal{D}}^{\alpha,r}$ is the differential matrix with components

$$\widetilde{\mathcal{D}}_{ij}^{\alpha,r} = (-\Delta)^{\alpha/2}\widetilde{H}_j(rx_i), \quad i,j = 0,...,N-1. \tag{3.14}$$

Then we need to deal with the fractional Laplacian of $\widetilde{H}_j\left(rx\right)$. By using together the scaling property of fractional Laplacian and the differential matrix formula in (3.7), we have the following matrix:

$$\begin{aligned}\widetilde{\mathcal{D}}_{ij}^{\alpha,r} &= (-\Delta)^{\alpha/2}\widetilde{H}_j(rx_i) \qquad\qquad (3.15)\\ &= \begin{cases} (2r)^{\alpha}\dfrac{(-1)^n\sqrt{(2n)!}}{2^n n!}\dfrac{\Gamma\left(n+\frac{\alpha}{2}+\frac{1}{2}\right)}{\Gamma\left(n+\frac{1}{2}\right)}{}_1F_1\left(n+\frac{\alpha}{2}+\frac{1}{2};\frac{1}{2};-z_i^2\right), \ j=2n; \\ 2^{\alpha+1}r^{\alpha}\dfrac{(-1)^n\sqrt{(2n+1)!}}{2^{n+\frac{1}{2}}n!}\dfrac{\Gamma\left(n+\frac{\alpha}{2}+\frac{3}{2}\right)}{\Gamma\left(n+\frac{3}{2}\right)}z_{i1}F_1\left(n+\frac{\alpha}{2}+\frac{3}{2};\frac{3}{2};-z_i^2\right), \ j=2n+1. \end{cases}\end{aligned}$$

where $z_i = rx_i$ for $i = 0, 1, ..., N-1$.

3.1.4 Applications to multi-term fractional PDEs

In this section, we claim that our spectral collocation method can be easily applied to the multi-term fractional PDEs. We shall still take the one-dimensional case as an example. Consider the following multi-term fractional PDEs

$$\sum_{j=1}^{J}(-\Delta)^{\alpha_j/2}u(x) = f(x), \quad x \in \mathbb{R}. \tag{3.16}$$

Note here the above problem is motivated by numerical methods for distributed order fractional models where the integral over order of the fractional differential equation is approximated using a quadrature rule, and then turned into multi-term problems, see e.g. [3, 15, 21, 50].

For the above multi-term models, by inserting the Hermite expansion (3.1) into the equation and imposing the collocation condition on Hermite Gauss points, one gets the following system:

$$\widetilde{\mathcal{D}}^{\mathcal{J}}\mathbf{c} = \mathbf{f} \qquad \text{with} \qquad \widetilde{\mathcal{D}}^{\mathcal{J}} = \sum_{j=1}^{J}\widetilde{\mathcal{D}}^{\alpha_j}. \tag{3.17}$$

Notice that the components of each differential matrix $\widetilde{\mathcal{D}}^{\alpha_j}$ can be computed by the explicit formula (3.7).

3.2 Generalized Hermite function $\{\widehat{H}_n(x)\}_n$

In the last section, we have proposed the spectral methods with the over-scaled bases $\{\widetilde{H}_n\}_n$. While the associated DM is easy to compute, its condition number grows fast with respect to the number of collocation points, and this is due to the poor property of the bases. In this section, we shall discuss the spectral collocation methods based on the generalized Hermite functions $\{\widehat{H}_n\}_n$ which are orthogonal with the weight function $\hat{\omega}(x) = 1$, and more widely studied. The main task is still to derive the explicit formula for the differential matrix involving the fractional Laplace operator.

3.2.1 The one dimensional case

The aim is the present the explicit formula for $\widehat{\mathcal{D}}^{\alpha}_{mn} = (-\Delta)^{\alpha/2}\widehat{H}_n(x_m)$. This also relies on the forward/inverse Fourier transform as done in the last section.

By the forward Fourier transform, we Notice that

$$\mathcal{F}\left\{\widehat{H}_n(x)\right\} = \frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}}\widehat{H}_n(x)e^{-\mathrm{i}\xi x}dx = (-\mathrm{i})^n\widehat{H}_n(\xi). \tag{3.18}$$

That is, the generalized Hermite functions $\left\{\widehat{H}_n(x)\right\}_n$ are eigenfunctions of the Fourier transform with eigenvalues $\{(-\mathrm{i})^n\}_n$, where $\mathrm{i} = \sqrt{-1}$.

A more difficult part is to compute the inverse Fourier transform. By the above fact and (1.5), we have to deal with the inverse fourier transform of $\left\{(-\mathrm{i})^n|\xi|^\alpha\widehat{H}_n(\xi)\right\}_n$. Notice that we can write

$$\widehat{H}_n(\xi) = \sum_{k=0}^{n}\hat{a}_{n,k}\exp(-\xi^2/2)\xi^k, \quad n = 0, 1, ..., N-1, \tag{3.19}$$

with $\widehat{a}_{n,k} = \frac{1}{\sqrt{2^n n!}}a_{n,k}$ for $k \le n$, where $a_{n,k}$ are the individual coefficients for Hermite polynomial as

$$H_n(\xi) = \sum_{k=0}^{n}a_{n,k}\xi^k.$$

And $a_{n,k}$ can be computed in a recursion way

$$\begin{aligned}
&a_{0,0} = 1,\ a_{1,0} = 0,\ a_{1,1} = 2;\\
&a_{n+1,k} = -a_{n,k+1}, \quad k = 0;\\
&a_{n+1,k} = 2a_{n,k-1} - (k+1)a_{n,k+1}, \quad k > 0.
\end{aligned}$$

Let us first consider the even terms with $k = 2m$, the inverse Fourier transform yields

$$\begin{aligned}
&\mathcal{F}^{-1}\left[\exp(-\xi^2/2)\xi^{2m}|\xi|^\alpha\right](x) \\
&= \frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}} \exp(-\xi^2/2)\xi^{2m}|\xi|^\alpha e^{\mathrm{i}\xi x} d\xi \\
&= \frac{2}{\sqrt{2\pi}}\int_{\mathbb{R}+} \exp(-\xi^2/2)\xi^{2m+\alpha}\cos(\xi x) d\xi \\
&= \frac{2^{\frac{2m+\alpha}{2}}}{\sqrt{\pi}}\Gamma\left(\frac{2m+1+\alpha}{2}\right) {}_1F_1\left(\frac{2m+1+\alpha}{2};\frac{1}{2};-\frac{x^2}{2}\right).
\end{aligned}$$

Then for the odd terms with $k = 2m+1$, it holds

$$\begin{aligned}
&\mathcal{F}^{-1}\left[\exp(-\xi^2/2)\xi^{2m+1}|\xi|^\alpha\right](x) \\
&= \frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}} \exp(-\xi^2/2)\xi^{2m+1}|\xi|^\alpha e^{\mathrm{i}\xi x} d\xi \\
&= \frac{2\mathrm{i}}{\sqrt{2\pi}}\int_{\mathbb{R}+} \exp(-\xi^2/2)\xi^{2m+1+\alpha}\sin(\xi x) d\xi \\
&= \frac{2^{\frac{2m+2+\alpha}{2}}\mathrm{i}}{\sqrt{\pi}}\Gamma\left(\frac{2m+3+\alpha}{2}\right) x\,{}_1F_1\left(\frac{2m+3+\alpha}{2};\frac{3}{2};-\frac{x^2}{2}\right).
\end{aligned}$$

For ease of notations, we denote

$$F_k(x) = \mathcal{F}^{-1}\left[\exp(-\xi^2/2)\xi^k|\xi|^\alpha\right](x), \quad k = 0, 1, ..., N-1.$$

Then by (3.19) the components of the differentiation matrix yield

$$\widehat{\mathcal{D}}^\alpha_{mn} = (-\Delta)^{\alpha/2}\widehat{H}_n(x_m) = (-\mathrm{i})^n \sum_{k=0}^{N-1} \hat{a}_{n,k} F_k(x_m), \quad 0 \le n, m \le N-1. \tag{3.20}$$

Notice that when $k > n$, we set $a_{n,k} = 0$.

In Fig. 3.2 we present the condition number of this differential matrix with respect to N. It is noticed from Fig. 3.2 that the condition number grows algebraically with expansion number N, much well behaved than the previous case where the over scaled bases are used. Moreover, the computation complexity of the DM above is almost the same as the formula (3.7) since the fractional Laplacian of generalized Hermite function is simply a evaluation of a linear combination of the confluent hypergeometric functions.

3.2.2 2D case

As in the former case for the over-scaled Hermite function $\widetilde{H}_n(x)$, the basis used for multi-dimension will be the tensorized 1D bases. We now consider the two di-

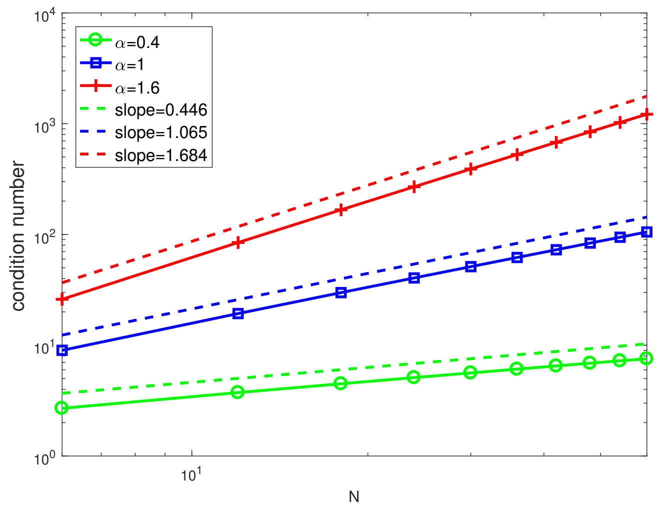

Figure 3.2: Condition number of the differentiation matrix for generalized Hermite function $\widehat{H}_n(x)$ versus N.

mensional case for the basis $\{\widehat{H}_n(x)\widehat{H}_m(y)\}_{n,m}$. First consider the forward Fourier transform we have

$$\begin{aligned}
\mathcal{F}\left[\widehat{H}_n\widehat{H}_m\right](\xi,\eta) &= \frac{1}{2\pi}\int_{\mathbb{R}}\int_{\mathbb{R}}\widehat{H}_n(x)\widehat{H}_m(y)e^{-\mathrm{i}x\xi}e^{-\mathrm{i}y\eta}dxdy \\
&= \frac{1}{2\pi}\int_{\mathbb{R}}\widehat{H}_n(x)e^{-\mathrm{i}x\xi}dx\int_{\mathbb{R}}\widehat{H}_m(y)e^{-\mathrm{i}y\eta}dy \\
&= (-\mathrm{i})^{n+m}\widehat{H}_n(\xi)\widehat{H}_m(\eta). \qquad (3.21)
\end{aligned}$$

Then, by the inverse Fourier transform we obtain

$$(-\Delta)^{\alpha/2}\left[\widehat{H}_n(x)\widehat{H}_m(y)\right] = \frac{(-\mathrm{i})^{n+m}}{(2\pi)}\int_{\mathbb{R}}\int_{\mathbb{R}}\left(\xi^2+\eta^2\right)^{\frac{\alpha}{2}}\widehat{H}_n(\xi)\widehat{H}_m(\eta)e^{\mathrm{i}x\xi}e^{\mathrm{i}y\eta}d\xi d\eta.$$

Similar as in the one dimensional case, we expand $H_n(\xi)H_m(\eta)$ as a combination of $\xi^k\eta^l$. Inspired by (3.19) we have

$$\widehat{H}_n(\xi)\widehat{H}_m(\eta) = \sum_{k=0}^{N-1}\sum_{l=0}^{N-1}\hat{a}_{n,k}\hat{a}_{m,l}\exp\left(-(\xi^2+\eta^2)/2\right)\xi^k\eta^l.$$

Next, we should deal with the inverse Fourier transform of terms like

$$\left(\xi^2+\eta^2\right)^{\frac{\alpha}{2}}\exp\left(-\left(\xi^2+\eta^2\right)/2\right)\xi^k\eta^l, \quad 0\le k,l\le N-1.$$

The derivation is similar as in the one dimensional case, and thus we omit the details here. To summarize, we introduce the matrix $F(\xi, \eta)$ as

$$F_{k,l} = \mathcal{F}^{-1}\left\{\left(\xi^2+\eta^2\right)^{\frac{\alpha}{2}} \exp\left(-(\xi^2+\eta^2)/2\right)\xi^k\eta^l\right\}$$
$$= \begin{cases} \dfrac{2^{\alpha/2}(-1)^{p+q}\Gamma(p+q+\frac{\alpha}{2}+1)\,{}_1F_1\left(p+q+\frac{\alpha}{2}+1; 2p+2q+1; -\frac{x^2+y^2}{2}\right)}{2^{p+q}\Gamma(2p+2q+1)}, & \\ \qquad k=2p,\ l=2q; & \\ \dfrac{2^{(\alpha+1)/2}(-1)^{p+q}i\Gamma(p+q+\frac{\alpha}{2}+2)y\,{}_1F_1\left(p+q+\frac{\alpha}{2}+2; 2p+2q+2; -\frac{x^2+y^2}{2}\right)}{2^{p+q}\Gamma(2p+2q+2)}, & \\ \qquad k=2p,\ l=2q+1; & \\ \dfrac{2^{(\alpha+1)/2}(-1)^{p+q}i\Gamma(p+q+\frac{\alpha}{2}+2)x\,{}_1F_1\left(p+q+\frac{\alpha}{2}+2; 2p+2q+2; -\frac{x^2+y^2}{2}\right)}{2^{p+q}\Gamma(2p+2q+2)}, & \\ \qquad k=2p+1,\ l=2q; & \\ \dfrac{-2^{\alpha/2+1}(-1)^{p+q}\Gamma(p+q+\frac{\alpha}{2}+3)xy\,{}_1F_1\left(p+q+\frac{\alpha}{2}+3; 2p+2q+3; -\frac{x^2+y^2}{2}\right)}{2^{p+q}\Gamma(2p+2q+3)}, & \\ \qquad k=2p+1,\ l=2q+1. & \end{cases}$$

Finally, we provide the explicit formula for the components of the differentiation matrix as follows

$$\begin{aligned} \widehat{\mathcal{D}}^{\alpha}_{(p-1)*N+q,(n-1)*N+m} &= (-\Delta)^{\alpha/2}\left\{\widehat{H}_n(x_p)\widehat{H}_m(y_q)\right\} \\ &= (-i)^{n+m}\sum_{k=0}^{N-1}\sum_{l=0}^{N-1}\hat{a}_{n,k}\hat{a}_{m,l}F_{k,l}(x_p,y_q). \end{aligned} \tag{3.22}$$

Remark 3.1 *Similar as in Section 3, for the spectral collocation methods with the generalized Hermite functions, one can easily include the scaling factors with slight modifications to the differential matrix. And furthermore, the application to multi-term fractional PDEs is also straightforward.*

3.3 Application to fractional differential equations

In the above sections, we have derived explicit formulas for the differential matrices by using the Hermite-type bases. In this section, we shall discuss the spectral collocation method with Lagrange type bases. For notation simplicity, we shall only present the one dimensional case. Notice that for this type of bases, we still search an approximated solution in the same finite space as in the above sections, however, such an approach indeed results in different differential matrices. By using the Lagrange type bases, we approximate the solution in the following way

$$u_N(x) = \sum_{j=0}^{N-1} u_j h_j(x), \quad \text{with} \quad h_j(x_k) = \delta_{jk}, \quad 0 \le j,k \le N-1.$$

Here the Lagrange type bases $\{h_j(x)\}_{j=0}^{N-1}$ are defined as

$$h_j(x) = \frac{e^{-x^2/2}}{e^{-x_j^2/2}} \prod_{i=0, i\neq j}^{N-1} \frac{x - x_j}{x_i - x_j}, \quad 0 \le j \le N-1.$$

The associated points $\{x_j\}_{j=0}^{N-1}$ are the Gauss-Hermite points. It is clear that we can express every Lagrange-type basis with the generalized Hermite functions, i.e.,

$$h_j(x) = \sum_{k=0}^{N-1} b_k^j \widehat{H}_k(x), \quad \text{with} \quad b_k^j = \frac{1}{\sqrt{\pi}} \widehat{H}_k(x_j)\, \hat{\omega}_j, \quad 0 \le j,k \le N-1.$$

where $\hat{\omega}_j$, $j = 0, 1, ..., N-1$ is the weights of the Gauss quadrature associated with the Hermite functions defined as:

$$\hat{\omega}_j = \frac{\sqrt{\pi}}{N \widehat{H}_{N-1}^2(x_j)}, \quad j = 0, 1, ..., N-1.$$

Consequently, we can easily derive the associated differential matrix $\widehat{D}^{L,\alpha}$ with Lagrange type bases

$$\widehat{D}_{i,j}^{L,\alpha} = (-\Delta)^{\alpha/2} h_j(x_i) = \sum_{k=0}^{N-1} b_k^j (-\Delta)^{\alpha/2} \widehat{H}_k(x_i). \tag{3.23}$$

The quantities $(-\Delta)^{\alpha/2} \widehat{H}_k(x_i)$ can be obtained via equation (3.20).

The condition number of the above differential matrix with respect to expansion number N is presented in Fig. 3.3. Again, we can see that the condition number grows algebraically with respect to expansion number N by N^α, in accordance of integer order differential equation, where the condition number for first and second order Hermite collocation methods are asymptotically N and N^2, as demonstrated in [89].

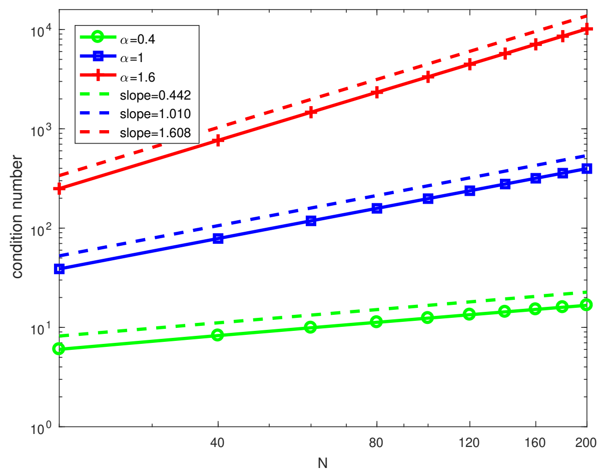

Figure 3.3: Condition number of the differentiation matrix for nodal expansion with the generalized Hermite function.

3.4 Convergence analysis

Let u and u_N be the solution of (1.3) and its collocation method with the differentiation matrix of the fractional Laplace operator given by $\widehat{D}^{L,\alpha}_{i,j}$ in (3.23), then we have the following theorem.

Theorem 3.3 *Assume that $u \in \hat{B}^{m_1}\left(\mathbb{R}^d\right)$ and $f \in \hat{B}^{m_2}\left(\mathbb{R}^d\right)$ with $m_1, m_2 > 0$, there exists an integer $N_0 > 0$, s.t. for $N > N_0$, we have*

$$\left\|u - u_N\right\| \leq \left\|u - u_N\right\|_{H^{\frac{\alpha}{2}}} \lesssim N^{\frac{d}{6}+\frac{\alpha/2-m_1}{2}}\left|u\right|_{\hat{B}^{m_1}\left(\mathbb{R}^d\right)} + N^{\frac{d}{6}-\frac{m_2}{2}}\left|f\right|_{\hat{B}^{m_2}\left(\mathbb{R}^d\right)} \tag{3.24}$$

Proof. For simplicity, we only prove the one dimensional case, higher dimension can be proved similarly. Recall that we collocate the equation on $N+1$ Hermite-Gauss points $\{x_j\}_{j=0}^N$ associated with the weight function $\hat{\omega}\left(x\right) = 1$.

$$(-\Delta)^{\alpha/2} u_N\left(x_j\right) + \rho u_N\left(x_j\right) = f\left(x_j\right), \quad j = 0, ..., N.$$

Multiply both sides with $v_N\left(x_j\right)\hat{\omega}_j$, where $v_N \in \hat{P}_N\left(\mathbb{R}\right)$, and sum up using the exactness of Hermite quadrature, we rewrite the scheme in the following variational form:

$$\left((-\Delta)^{\alpha/2} u_N, v_N\right)_N + \rho\left(u_N, v_N\right) = \left(\hat{I}^h_N f, v_N\right). \tag{3.25}$$

where

$$\left(u_N, v_N\right)_N = \sum_{j=0}^{N} (-\Delta)^{\alpha/2} u_N\left(x_j\right) v_N\left(x_j\right)\hat{\omega}_j.$$

Note that

$$\left((-\Delta)^{\alpha/2} v_N, v_N\right)_N \approx \left((-\Delta)^{\alpha/2} v_N, v_N\right)$$

and

$$\left((-\Delta)^{\alpha/2} v_N, v_N\right) = \left(|\xi|^\alpha \hat{v}_N, \hat{v}_N\right) \geq 0.$$

So there exists an integer $N_0 > 0$, such that for all $N > N_0$, we have

$$\left((-\Delta)^{\alpha/2} v_N, v_N\right)_N \geq 0, \forall v_N \in \hat{P}_N\left(\mathbb{R}\right).$$

Define the bilinear form

$$a_\alpha\left(u, v\right) = \left((-\Delta)^{\alpha/2} u, v\right) + \rho\left(u, v\right).$$

Then for $N \geq N_0$, we have $a_\alpha\left(u, u\right) \geq 0$. Define the norm

$$\|u\|_\alpha := \sqrt{a_\alpha\left(u, u\right)}.$$

By definition, we have

$$\|u\|^2 \leq a_\alpha\left(u, u\right) \lesssim \|u\|^2_{H^{\frac{\alpha}{2}}}.$$

Rewrite the variation formin (3.25)

$$\begin{aligned}\left((-\Delta)^{\alpha/2} u_N, v_N\right) &+\rho\left(u_N, v_N\right) = \\ &\left(\hat{I}^h_N f, v_N\right) + \left((-\Delta)^{\alpha/2} u_N - \hat{I}^h_N\left((-\Delta)^{\alpha/2} u_N\right), v_N\right)\end{aligned} \tag{3.26}$$

Compare (3.25) with the variational form of (1.3)

$$\left((-\Delta)^{\alpha/2} u, v_N\right) + \rho\left(u, v_N\right) = \left(f, v_N\right), \tag{3.27}$$

and apply the Strang's first lemma 2.8, we obtain immediately

$$\left\|u - u_N\right\|_\alpha \lesssim \inf_{v_N \in \hat{P}_N} \left\|u - v_N\right\|_\alpha + \left\|(-\Delta)^{\alpha/2} u - \hat{I}^h_N\left((-\Delta)^{\alpha/2} u\right)\right\| + \left\|f - \hat{I}^h_N f\right\|$$

Since

$$\inf_{v_N \in \hat{P}_N} \left\|u - v_N\right\|_\alpha \leq \left\|u - \hat{I}^h_N u\right\|_\alpha \lesssim \left\|u - \hat{I}^h_N u\right\|_{H^{\frac{\alpha}{2}}}$$

and

$$\begin{aligned}(-\Delta)^{\alpha/2} u - \hat{I}^h_N\left((-\Delta)^{\alpha/2} u\right) &= \left((-\Delta)^{\alpha/2} u + cu\left(x\right)\right) - \hat{I}^h_N\left((-\Delta)^{\alpha/2} u + \rho u\left(x\right)\right) \\ &+ \rho\left(u - \hat{I}^h_N u\right) = f - \hat{I}^h_N f + \rho\left(u - \hat{I}^h_N u\right)\end{aligned}$$

Using lemma 2.3, we have the desired result.

3.5 Numerical examples

In this chapter, we shall present several constructive examples to show the convergence property of our spectral collocation methods. We first present the convergence property of spectral collocation methods with over-scaled Hermite function $\widetilde{H}_n(x)$ and generalized Hermite function $\widehat{H}_n(x)$. In all our computations, we shall report the numerical error both in the weighted norm e_w and in the maximum norm e_m, which are defined respectively in this section as

$$e_w = \|u(x) - u_N(x)\|_\omega^2, \quad e_m = \max_j |u(x_j) - u_N(x_j)|.$$

Here $\omega(x) = e^{x^2}$ for the bases $\{\widetilde{H}_n(x)\}_n$ and $\omega(x) = 1$ for the generalized Hermite functions $\{\widehat{H}_n(x)\}_n$.

3.5.1 The fractional Laplace equation

Our first example is the fractional Laplace equation

$$\begin{cases} (-\Delta)^{\alpha/2} u(x) = f(x), & x \in \mathbb{R}, \\ u(x) = 0, & |x| \to \infty. \end{cases} \tag{3.28}$$

The right hand side is chosen such that the exact solution is $u(x) = \exp(-x^2)\sin x$. Notice that for a given exact solution $u(x)$, the right hand side does not necessary have explicit formula, and in such cases, we shall compute it by expanding $u(x)$ with a large enough number of the basis functions. This is also true for all other examples.

We perform computations with different fractional order, i.e., $\alpha = 0.4$, 1 and 1.6. The numerical errors against the numerical of points N with the over scaled bases and the generalized Hermite functions are presented in Fig. 3.4 and Fig. 3.5, respectively. For the over-scaled bases, no scaling factor is needed, i.e, $r = 1$, while for the generalized Hermite functions, we choose $r = \sqrt{2}$. In Fig. 3.4 and Fig. 3.5, the numerical error in weighted norm and in maximum norm are reported in the left plot and right plot, respectively. It is clear that spectral convergence is obtained for all cases of α. While no scaling factor is needed for the over scaled bases, it is noticed that the convergence is polluted when a larger number of collocation points are used, due to the fast grow of the condition number.

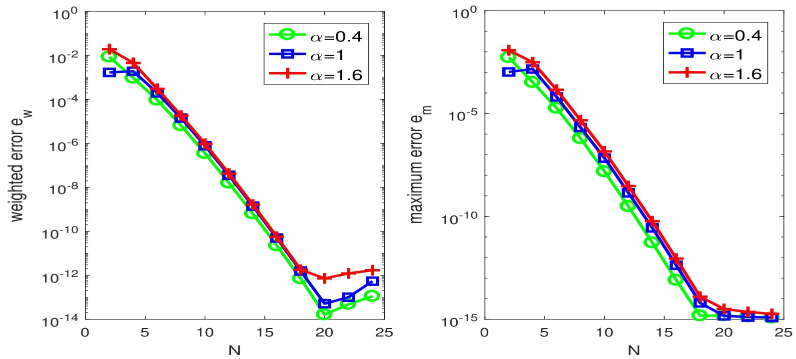

Figure 3.4: Numerical error with the over-scaled bases with $u(x) = \exp(-x^2)\sin x$. Left: weighted norm. Right: maximum norm.

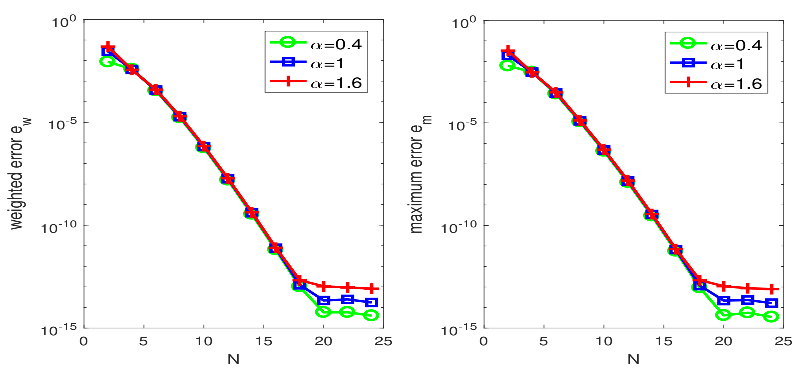

Figure 3.5: Numerical error with the generalized Hermite functions with $u(x) = \exp(-x^2)\sin x$. Left: weighted norm. Right: maximum norm.

3.5.2 A linear fractional PDE

Next, we consider the following fractional PDE

$$\begin{cases} (-\Delta)^{\alpha/2}u\,(x) + 2u\,(x) = f\,(x)\,, & x \in \mathbb{R} \\ u\,(x) = 0, & x \to \infty \end{cases} \tag{3.29}$$

We first test the performance of the over-scaled bases. To this end, we set $u(x) = \exp(-\frac{x^2}{2})x^2\cos(x)$, and the right hand side can be computed accordingly. Again, we consider $\alpha = 0.4, 1$ and 1.6. The numerical results with a scaling factor $r = 1/\sqrt{2}$ and without the scaling factor ($r = 1$) are reported in Fig. 3.6 and Fig. 3.7, respectively. It is clear seen that using a proper scaling factor results in faster convergence rate for both the weighted error and the maximum error.

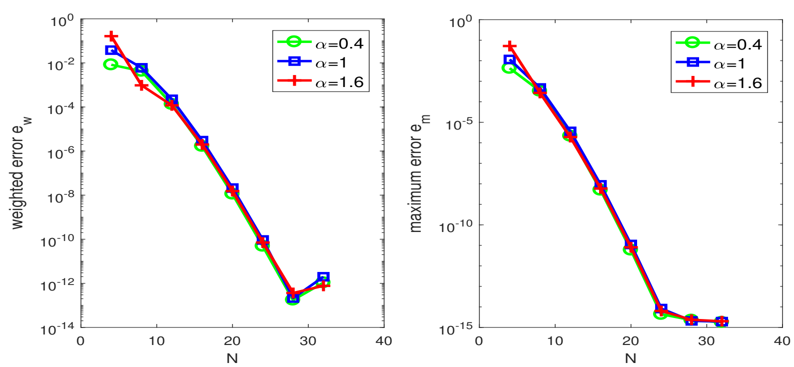

Figure 3.6: Numerical error with the over scaled bases for exact solution $u(x) = \exp(-\frac{x^2}{2})x^2\cos(x)$. The scaling factor is $r = 1/\sqrt{2}$. Left: weighted norm. Right: maximum norm.

Now we test the generalized Hermite functions. For the same equation we choose the right hand side such that the solution yields $u(x) = \exp(-2x^2)x^2\cos(x)$. It is clear that the optimal scaling factor is $r = 2$. The numerical results with a scaling factor $r = 2$ and without a scaling factor (i.e., $r = 1$) are reported Fig. 3.8 and Fig. 3.9, respectively. Again, it is shown that a proper scaling factor can be useful to speed up the convergence.

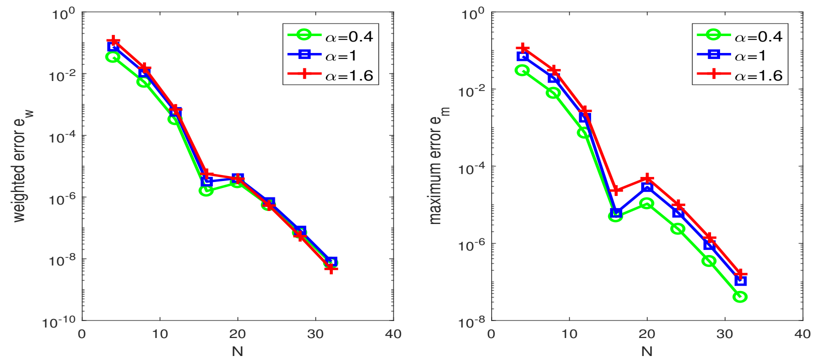

Figure 3.7: Numerical error with the over scaled bases for exact solution $u(x) = \exp(-\frac{x^2}{2})x^2\cos(x)$. The scaling factor is $r = 1$. Left: weighted norm. Right: maximum norm.

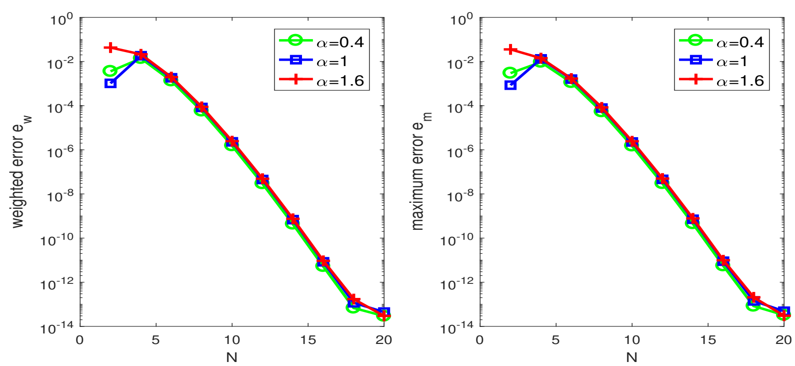

Figure 3.8: Numerical error with the generalized Hermite functions for exact solution $u(x) = \exp(-2x^2)x^2\cos(x)$. The scaling factor is chosen as $r = 2$. Left: weighted norm. Right: maximum norm.

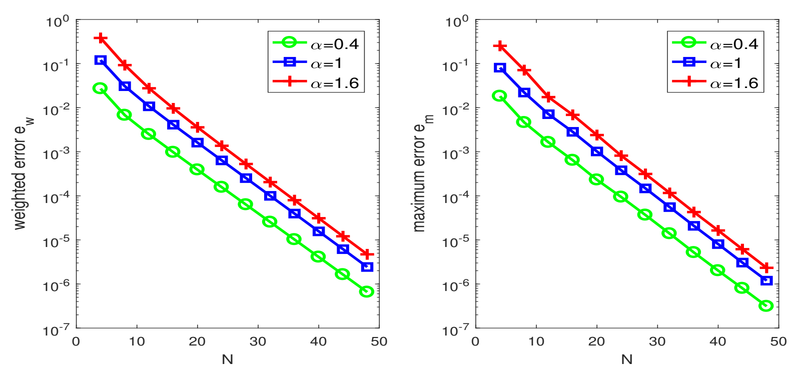

Figure 3.9: Numerical error with generalized Hermite functions for with exact solution $u(x) = \exp(-2x^2)x^2\cos(x)$. The scaling factor is chosen as $r = 1$. Left: weighted norm. Right: maximum norm.

3.5.3 A two-dimensional example

We now consider a two dimensional example, and the equation considered is

$$(-\Delta)^{\alpha/2}u(x,y) + 2u(x,y) = f(x,y). \tag{3.30}$$

The exact solution is chosen as $u(x,y) = \exp(-(x^2+y^2))\sin(x+y)$. We also perform the computations with $\alpha = 0.4$, 1 and 1.6. To avoid too much pictures, here we only test the performance of the over-scaled bases. The numerical errors in weighted and maximum norm against the numerical of number of collocation points N are presented in Fig. 3.10. Spectral convergence is again observed.

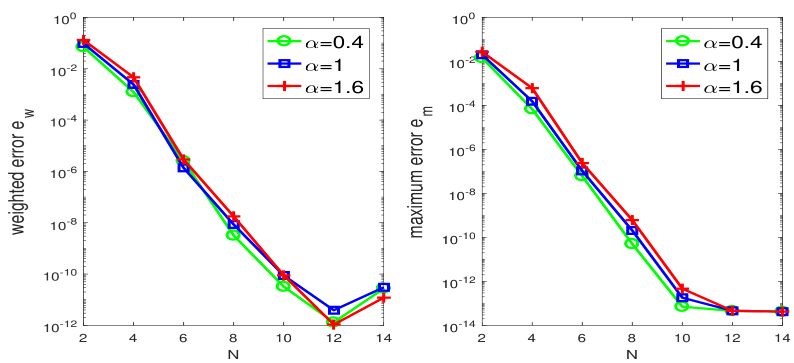

Figure 3.10: Numerical error for a two dimensional example with the exact solution $u(x,y) = \exp(-(x^2+y^2))\sin(x+y)$. Left: weighted norm. Right: maximum norm.

3.5.4 A multi-term fractional model

Our next example the multi-term Laplacian equation:

$$\sum_{j=1}^{J}(-\Delta)^{\alpha_j/2}u(x) = f(x), \quad x \in \mathbb{R}. \tag{3.31}$$

Here we set $J = 4$ and $\{\alpha_j\}_{j=1}^{J}$ are chosen as the transformed Legendre-Gauss points:

$$\alpha_1 = 0.139, \quad \alpha_2 = 0.660, \quad \alpha_3 = 1.340, \quad \alpha_4 = 1.861. \tag{3.32}$$

We set the exact solution to be $u(x) = \exp(-3x^2/2)(\sin x + x^6 + x^2\cos x)$ and the right hand side can be computed accordingly. Again, we test the performance of the over-scaled bases. In this example, we consider scaling factors $r = \sqrt{1.5}$, $\sqrt{1.3}$, and

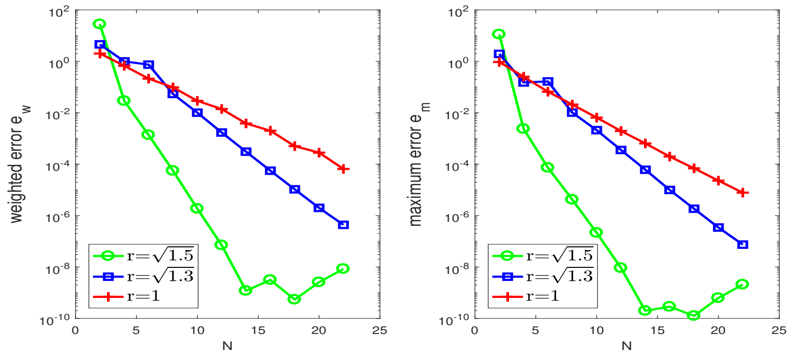

Figure 3.11: Numerical error for the multi-term fractional Laplace equation with exact solution $u(x) = e^{-3x^2/2}(\sin x + x^6 + x^2 \cos x)$. Left: weighted norm. Right: maximum norm.

the approach without a scaling factor, i.e., $r = 1$. The corresponding numerical results are reported in Fig. 3.11. We can see that both the weighted error and maximum error decay fast for the case of $r = \sqrt{1.5}$. And this indicates the effectiveness of using a scaling in improving convergence rate.

3.5.5 A nonlinear example

Our next example is a nonlinear fractional PDE

$$(-\Delta)^{\alpha/2} u(x) + u^2(x) = g(x) \tag{3.33}$$

For the over scaled bases $\widetilde{H}_n(x)$, we set the exact solution as $u(x) = \exp(-x^2)(\sin(x)+x^2)$. For the generalized Hermite functions $\widehat{H}_n(x)$, the exact solution is chose to be $u(x) = \exp(-x^2/2)(\sin(x) + x^2)$. In our computations, for each expansion number N, we use the Newton iteration method with a tolerance 10^{-16} to deal with the nonlinear term. The performance of the two types of spectral collocation methods are presented in Fig. 3.12 and Fig. 3.13, respectively. In both cases, spectral convergence rates are obtained.

3.5.6 An eigenvalue problem

Finally we consider the following eigenvalues problem

$$\left((-\Delta)^{\alpha/2} + x^2\right) u(x) = \lambda u(x) \tag{3.34}$$

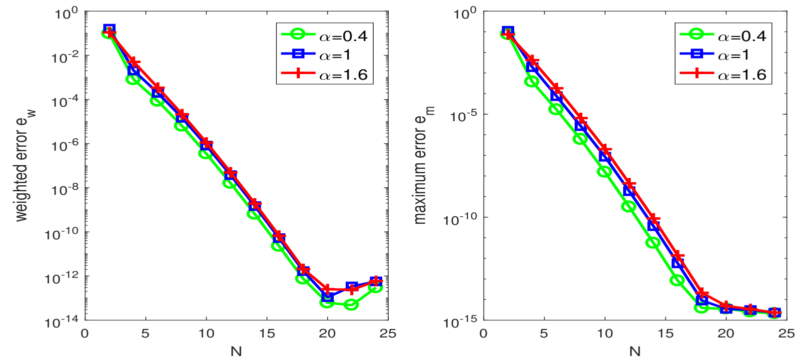

Figure 3.12: Numerical error with $\widetilde{H}_n$ for the nonlinear problem. Left: weighted norm. Right: maximum norm.

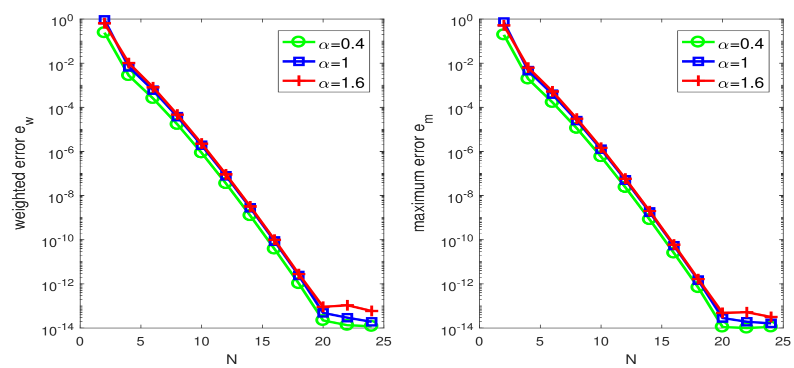

Figure 3.13: Numerical error with $\widehat{H}_n$ for the nonlinear problem. Left: weighted norm. Right: maximum norm.

The above eigenvalue problem with $\alpha = 1$ has been analyzed in [42]. In particular, the eigenvalues of this problems is given by

$$\lambda_{2k-1} = -a'_k, \quad \lambda_{2k} = -a_k, \quad k = 1, 2, ...,$$

where a_k and a'_k are the roots of the following Airy function and its derivative (in the decreasing order)

$$A(x) = \frac{1}{\pi} \int_0^\infty \cos\left(\frac{t^3}{3} + xt\right) dt.$$

In this example, we shall compute the first three eigenvalues by the spectral collocation method. The exact eigenvalues are

$$\lambda_1 \approx 1.01879297164747, \quad \lambda_2 \approx 2.33810741045976, \quad \lambda_3 \approx 3.24819758217983.$$

Numerical result are presented in Fig. 3.14 with semilogy scale. An algebraic decay is observed and this is due to the algebraic decay (non-exponential decay) of eigenvalues.

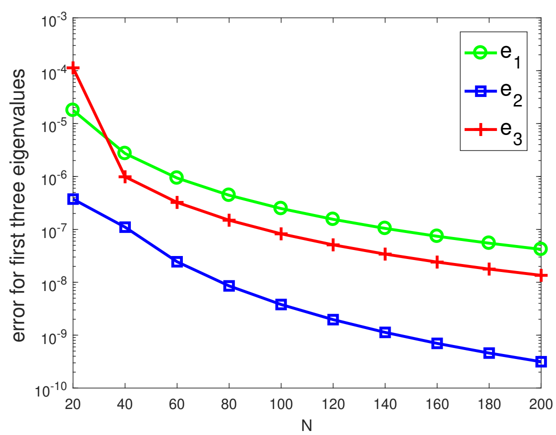

Figure 3.14: Numerical errors of the first three eigenvalue with generalized Hermite function.

3.6 Concluding remarks

In this chapter, we proposed the spectral collocation method with two kinds of hermite functions, namely, the over-scaled Hermite functions and generalized Hermite functions. For both approaches, explicit formula for the differentiation matrices are derived. To deal with solutions with fast or slow decay rate, a scaling factor in spectral implementation is discussed.

Although the numerical experiments indicate the spectral rate of convergence, there are still several issues requiring future investigations:

- For over-scaled Hermite functions (which was used extensively in physics, see [67]) the condition numbers of the associated matrices grow very fast with respect to the number of collocation points N. Thus, it is useful to investigate some efficient pre-conditioners in this case.

- We only provide some ad-hoc discussions on the scaling factors. It will be more meaningful to provide some more practical guidance on the optimal choice of the scaling factors, see, e.g., [53].

Chapter 4

Modified rational spectral collocation methods

In this chapter, we propose spectral collocation method with the modified rational function defined in (2.35). In the last chapter, we already have constructed the spectral collocation method based on Hermite function, which is a good choice for solutions that decay exponentially in infinity. However, this is not always the case for solutions of fractional differential equations. The solutions are sometimes non-exponential with heavy tails, which may be hard to be approximated by Hermite functions, even with scaling. Such situations occur in evolution equations like the fractional porous medium equation, for example, in [9, 14, 61] or fractal Burgers equation in [8, 82]. In these problems solutions often develop an algebraic tail and not suitable to approximate with Hermite functions.

An effective and common way in dealing with unbounded domain is to use a suitable mapping to transform an infinite domain to a finite domain, where the images of classical orthogonal functions in finite domain can be used to approximate solutions of differential equations in infinite domain, studied in [10, 33, 35, 85, 87]. Let

$$t \in I = [-1, 1]\,, \quad x \in \Lambda := (0, +\infty) \;\text{ or }\; (-\infty, +\infty)\,.$$

Jacobi polynomials defined on I can be utilized to form the so-called mapped Jacobi polynomials which are orthogonal functions on infinite domain. In order to transform from finite domain to infinite domain, several typical mappings can be used, for example, algebraic, logarithmic, or exponential mappings. The special feature which distinguishes these mapping is that as $t \to \pm 1$, x varies algebraically, logarithmically, or exponentially for corresponding mappings. In this chapter, we are dealing with solutions of slow decay rate, and then following algebraic mapping is used.

$$
\begin{aligned}
t &= \frac{x}{\sqrt{1+x^2}}, \quad x = \frac{t}{\sqrt{1-t^2}}, \quad \text{for the whole line.}\\
t &= \frac{x-1}{x+1}, \qquad x = \frac{1+t}{1-t}, \qquad \text{for the half line.}
\end{aligned}
$$

And different from Hermite-Gauss points which are more evenly distributed, mapped Jacobi-Gauss points are more clustered near origin and spread further, and thus a much larger effective interval is covered.

After we have got the orthogonal functions in infinite domain– mapped Jacobi polynomials or rational functions, and approximation result in certain Hilbert spaces, we can directly construct spectral methods in unbounded domain. However, the mapped Jacobi polynomials are mutually orthogonal in a weighted Sobolev space. The non-uniform weights in the standard rational approximations may bring in some difficulties for certain problems which are only well-posed in non-weighted Sobolev spaces. And the appearance of non-uniform weights may destroy the conservation properties for the numerical solutions. To remedy this deficiency, modified Legendre rational functions for spectral approximation on the half line and whole line are proposed separately in [88] and [32]. Also a modified Chebyshev rational method is developed in [34], in which fast transforms are possble than to FFT.

Here we generalize the modified Legendre rational functions and modified Chebyshev rational functions by introducing the modified rational function $R_n^{\lambda}(x)$ on the whole unbounded domain. Before computing the fractional Laplacian of modified rational functions, we first give the result for some simple functions. Here "simple" functions stand for $\dfrac{1}{(1+x^2)^{\gamma}}$ and $\dfrac{x}{(1+x^2)^{\gamma+\frac{1}{2}}}$ for $r > 0$.

4.1 Computing fractional Laplacian with simple functions

Before computing the fractional Laplacian of modified rational functions, we first give in the following theorem of the fractional Laplacian of $\dfrac{1}{(1+x^2)^{\gamma}}$ and then use the definition via Fourier transform in (1.5) to prove this.

Theorem 4.1

$$(-\Delta)^{\alpha/2}\left\{\frac{1}{(1+x^2)^\gamma}\right\} = \frac{2^\alpha\Gamma\left(\frac{\alpha}{2}+\gamma\right)\Gamma\left(\frac{1+\alpha}{2}\right)}{\Gamma\left(\frac{1}{2}\right)\Gamma(\gamma)}\,{}_2F_1\left(\frac{\alpha}{2}+\gamma,\frac{1+\alpha}{2};\frac{1}{2};-x^2\right). \tag{4.1}$$

Proof. First using (2.20) we have

$$u(x) = \frac{1}{(1+x^2)^\gamma} = {}_2F_1\left(\gamma,\frac{1}{2};\frac{1}{2};-x^2\right).$$

Then for the Fourier transform part

$$\begin{aligned}
\hat{u}(\xi) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\frac{e^{-ix\xi}}{(1+x^2)^\gamma}dx = \frac{2}{\sqrt{2\pi}}\int_0^\infty\frac{\cos(x\xi)}{(1+x^2)^\gamma}dx\\
&= \sqrt{\frac{2}{\pi}}\int_0^\infty \cos(x\xi)\,{}_2F_1\left(\gamma,\frac{1}{2};\frac{1}{2};-x^2\right)dx\\
&= \begin{cases} for\ \xi\geq 0: \sqrt{2\pi}2^{-\gamma+\frac{1}{2}}\xi^{\gamma-\frac{1}{2}}\dfrac{K_{\gamma-\frac{1}{2}}(\xi)}{\Gamma(\gamma)\Gamma\left(\frac{1}{2}\right)}.\\ for\ \xi<0: \sqrt{2\pi}2^{-\gamma+\frac{1}{2}}(-\xi)^{\gamma-\frac{1}{2}}\dfrac{K_{\gamma-\frac{1}{2}}(-\xi)}{\Gamma(\gamma)\Gamma\left(\frac{1}{2}\right)}.\end{cases}
\end{aligned}$$

For the inverse Fourier transform part we have

$$\begin{aligned}
\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}e^{ix\xi}|\xi|^\alpha\hat{u}(\xi)\,d\xi &= \frac{2^{-\gamma+\frac{3}{2}}}{\Gamma(\gamma)\Gamma\left(\frac{1}{2}\right)}\int_0^\infty\cos(x\xi)\,\xi^{\alpha+\gamma-\frac{1}{2}}K_{\gamma-\frac{1}{2}}(\xi)\,d\xi\\
&= \frac{2^\alpha\Gamma\left(\frac{\alpha}{2}+\gamma\right)\Gamma\left(\frac{1+\alpha}{2}\right)}{\Gamma\left(\frac{1}{2}\right)\Gamma(\gamma)}\,{}_2F_1\left(\frac{\alpha}{2}+\gamma,\frac{1+\alpha}{2};\frac{1}{2};-x^2\right).
\end{aligned}$$

This completes the proof. □

Using similar argument, for $\dfrac{x}{(1+x^2)^{\gamma+\frac{1}{2}}}$ we have the following theorem

Theorem 4.2

$$(-\Delta)^{\alpha/2}\left\{\frac{x}{(1+x^2)^{\gamma+\frac{1}{2}}}\right\} = \frac{2^\alpha\Gamma\left(\frac{\alpha+1}{2}+\gamma\right)\Gamma\left(\frac{3+\alpha}{2}\right)}{\Gamma\left(\frac{3}{2}\right)\Gamma\left(\gamma+\frac{1}{2}\right)}x\,{}_2F_1\left(\frac{\alpha+1}{2}+\gamma,\frac{3+\alpha}{2};\frac{3}{2};-x^2\right). \tag{4.2}$$

Proof. For the Fourier transform part, we use (2.20) then

$$u(x) = \frac{x}{(1+x^2)^{\gamma+\frac{1}{2}}} = x\,{}_2F_1\left(\gamma+\frac{1}{2},\frac{3}{2};\frac{3}{2};-x^2\right)$$

Then for the Fourier transform part

$$\hat{u}(\xi) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{xe^{-ix\xi}}{(1+x^2)^{\gamma+\frac{1}{2}}} dx = \frac{-2i}{\sqrt{2\pi}} \int_{0}^{\infty} \frac{x\sin(x\xi)}{(1+x^2)^{\gamma+\frac{1}{2}}} dx$$

$$= -i\sqrt{\frac{2}{\pi}} \int_0^{\infty} x\sin(x\xi)\, {}_2F_1\left(\gamma+\frac{1}{2}, \frac{3}{2}; \frac{3}{2}; -x^2\right) dx$$

$$= \begin{cases} for\xi \geq 0 : -i\sqrt{2\pi}2^{-\gamma-1}\xi^{\gamma} \frac{K_{\gamma-1}(\xi)}{\Gamma\left(\gamma+\frac{1}{2}\right)\Gamma\left(\frac{3}{2}\right)} \\ for\xi < 0 : i\sqrt{2\pi}2^{-\gamma-1}(-\xi)^{\gamma} \frac{K_{\gamma-1}(-\xi)}{\Gamma\left(\gamma+\frac{1}{2}\right)\Gamma\left(\frac{3}{2}\right)} \end{cases}$$

For the inverse Fourier transform part

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ix\xi} |\xi|^{\alpha} \hat{u}(\xi)\, d\xi$$

$$= \frac{2^{-\gamma}}{\Gamma\left(\gamma+\frac{1}{2}\right)\Gamma\left(\frac{3}{2}\right)} \int_0^{\infty} \sin(x\xi)\, \xi^{\alpha+\gamma} K_{\gamma-1}(\xi)\, d\xi$$

$$= \frac{2^{\alpha}\Gamma\left(\frac{\alpha+1}{2}+\gamma\right)\Gamma\left(\frac{3+\alpha}{2}\right)}{\Gamma\left(\frac{3}{2}\right)\Gamma\left(\gamma+\frac{1}{2}\right)} x\, {}_2F_1\left(\frac{\alpha+1}{2}+\gamma, \frac{3+\alpha}{2}; \frac{3}{2}; -x^2\right)$$

This completes the proof. □

Remark 4.1 *From* (4.1) *and* (4.2), *we observe that even with different* γ, *the second and third parameters of the hypergeometric functions are the same, and this provides a convenience for the adoption of the recurrence relation in* (2.22) *which we will demonstrate later.*

4.2 Computing with modified rational functions

In this section, we compute the fractional Laplacian of the modified rational functions R_n^{λ} defined in (2.35). For convenience, let $\beta = \frac{\lambda+1}{2}$. In former sections, we already know $R_{2n}^{\lambda}(x)$ is a finite sum of

$$\frac{1}{(1+x^2)^{k+\beta}}, \quad where \quad k = 0, 1, ..., n.$$

Then for even terms $R_{2n}^{\lambda}(x)$, we need to compute a finite sum of the fractional laplacian of these simple functions which is already known. Let $\gamma = k+\beta$ in (4.1), the fractional Laplacian of the even term of the modified rational functions are a finite sum of terms

$$\frac{2^{\alpha}\Gamma\left(\frac{\alpha}{2}+\beta+k\right)\Gamma\left(\frac{1+\alpha}{2}\right)}{\Gamma\left(\frac{1}{2}\right)\Gamma(k+\beta)} {}_2F_1\left(\frac{\alpha}{2}+\beta+k, \frac{1+\alpha}{2}; \frac{1}{2}; -x^2\right), \quad where \quad k = 0, 1, ..., n.$$

More specifically from (2.37) we have

Theorem 4.3

$$(-\Delta)^{\alpha/2} R_{2n}^{\lambda}(x) = \frac{2^{\alpha}\Gamma\left(\frac{1+\alpha}{2}\right)}{\Gamma\left(\frac{1}{2}\right)} \frac{(\lambda)_n}{(1)_n} \frac{\left(\lambda+\frac{1}{2}\right)_n}{\left(\frac{1}{2}\right)_n} \frac{\Gamma\left(\frac{\alpha}{2}+\beta\right)}{\Gamma(\beta)}$$
$$\sum_{k=0}^{n} \frac{(-n)_k (n+\lambda)_k}{\left(\lambda+\frac{1}{2}\right)_k k!} \frac{\left(\frac{\alpha}{2}+\beta\right)_k}{(\beta)_k} {}_2F_1\left(\frac{\alpha}{2}+\beta+k, \frac{1+\alpha}{2}; \frac{1}{2}; -x^2\right). \tag{4.3}$$

Similarly for odd $R_{2n+1}^{\lambda}(x)$, let $\gamma = k+\beta+\frac{1}{2}$ in (4.2), we have the following theorem:

Theorem 4.4

$$(-\Delta)^{\alpha/2} R_{2n+1}^{\lambda}(x) = \frac{2^{\alpha}\Gamma\left(\frac{3+\alpha}{2}\right)}{\Gamma\left(\frac{3}{2}\right)} \frac{2\lambda(\lambda+1)_n}{(1)_n} \frac{\left(\lambda+\frac{1}{2}\right)_n}{\left(\frac{3}{2}\right)_n} \frac{\Gamma\left(\frac{\alpha+1}{2}+\beta\right)}{\Gamma\left(\frac{1}{2}+\beta\right)}$$
$$x\sum_{k=0}^{n} \frac{(-n)_k (n+\lambda+1)_k}{\left(\lambda+\frac{1}{2}\right)_k k!} \frac{\left(\frac{\alpha+1}{2}+\beta\right)_k}{\left(\frac{1}{2}+\beta\right)_k} {}_2F_1\left(\frac{\alpha+1}{2}+\beta+k, \frac{3+\alpha}{2}; \frac{3}{2}; -x^2\right). \tag{4.4}$$

Remark 4.2 *We observe from* (4.3) *and* (4.4) *that the fractional Laplacian of the modified rational functions we chose are a finite sum of hypergeometric functions. For even terms, the second and third parameters of the hypergeometric functions are always the same, while the first parameter increases by 1 each time, hence using* (2.22)*, the result can be computed quickly in a recurrent way. This also applies to the odd terms.*

Remark 4.3 *Note here we can also using the scaling parameter* $s > 0$*, as introduced in [74], where the algebraic mapping in* (2.34) *turns to*

$$x = \frac{st}{\sqrt{1-t^2}}, \quad t = \frac{x}{\sqrt{s^2+x^2}}.$$

The corresponding modified rational function can be defined as

$$R_{n,s}^{\lambda}(x) := \frac{1}{(s^2+x^2)^{\frac{\lambda+1}{2}}} C_n^{\lambda}\left(\frac{x}{\sqrt{s^2+x^2}}\right).$$

Comparing with (2.35)*, we have*

$$R_{n,s}^{\lambda}(x) = s^{\lambda+1} R_n^{\lambda}\left(\frac{x}{s}\right).$$

Using this scaling property, we can easily compute the fractional Laplacian of $R_{n,s}^{\lambda}(x)$*. As is demonstrated in [74], the mapping parameter* s *affects the distribution of the Gauss nodes, and thus the effective interval. For simplicity, here we omit further information for* s*.*

4.3 Application to fractional differential equations

In this section, we consider the spectral method based on the $\left\{R_n^\lambda(x)\right\}_n$. We assume that the solution admits an algebraic decay in infinity, and approximate $u(x)$ with a finite sum of the the basis $\{R_n^\lambda(x)\}_n$. i.e.,

$$u(x) \approx u_N(x) = \sum_{n=0}^{N-1} c_n R_n^\lambda(x). \tag{4.5}$$

By inserting the above expansion into the fractional PDE (1.3), we obtain

$$\sum_{n=0}^{N-1} c_n(-\Delta)^{\alpha/2} R_n^\lambda(x) + \rho \sum_{n=0}^{N-1} c_n R_n^\lambda(x) = f(x), x \in \mathbb{R}. \tag{4.6}$$

Let $x_i = \frac{t_i}{\sqrt{1-t_i^2}}, i = 0, 1, ..., N-1$, where $\{t_i\}_{i=0}^{N-1}$ are the roots of the N-th order Gegenbauer polynomial $C_N^\lambda(t)$, we then impose the collocation conditions on these collocation points, which yields

$$\sum_{n=0}^{N-1} c_n(-\Delta)^{\alpha/2} R_n^\lambda(x_i) + \rho \sum_{n=0}^{N-1} c_n R_n^\lambda(x_i) = f(x_i), \quad i = 0, 1, ..., N-1.$$

Then we can write the above equations into the following system

$$\mathcal{D}^{\alpha,\lambda}\mathbf{c} + \rho\mathcal{R}^\lambda\mathbf{c} = \mathbf{f},$$

where $\mathbf{c} = (c_0, ..., c_{N-1})^T$ is the unknown coefficient vector, and $\mathcal{D}^{\alpha,\lambda} \in \mathbb{R}^{N\times N}$ is the differential matrix with components

$$\mathcal{D}_{i,j}^{\alpha,\lambda} = (-\Delta)^{\alpha/2} R_j^\lambda(x_i), \quad i, j = 0, 1, ..., N-1.$$

By solving the above linear system one gets an approximated solution $u_N(x)$. From (4.3) and (4.4), we have the components of the differentiation matrix of pseudo-spectral method as

$$D_{i,j}^{\alpha,\lambda} = \begin{cases} \frac{2^\alpha \Gamma\left(\frac{1+\alpha}{2}\right)}{\Gamma\left(\frac{1}{2}\right)} \frac{(\lambda)_n}{(1)_n} \frac{\left(\lambda+\frac{1}{2}\right)_n}{\left(\frac{1}{2}\right)_n} \sum_{k=0}^{n} \frac{(-n)_k (n+\lambda)_k}{\left(\lambda+\frac{1}{2}\right)_k k!} \frac{\Gamma\left(\frac{\alpha}{2}+\beta+k\right)}{\Gamma(k+\beta)} {}_2F_1\left(\frac{\alpha}{2}+\beta+k, \frac{1+\alpha}{2}; \frac{1}{2}; -x_i^2\right), \\ \qquad j = 2n; \\ \frac{2^\alpha \Gamma\left(\frac{3+\alpha}{2}\right)}{\Gamma\left(\frac{3}{2}\right)} \frac{2\lambda(\lambda+1)_n}{(1)_n} \frac{\left(\lambda+\frac{1}{2}\right)_n x_i}{\left(\frac{3}{2}\right)_n} \sum_{k=0}^{n} \frac{(-n)_k (n+\lambda+1)_k}{\left(\lambda+\frac{1}{2}\right)_k k!} \frac{\Gamma\left(\frac{\alpha+1}{2}+\beta+k\right)}{\Gamma\left(\frac{1}{2}+\beta+k\right)} {}_2F_1\left(\frac{\alpha+1}{2}+\beta+k, \frac{3+\alpha}{2}; \frac{3}{2}; -x_i^2\right), \\ \qquad j = 2n+1. \end{cases} \tag{4.7}$$

In Fig.4.1, we present the condition number of this differential matrix with respect to the number of collocation points N, and test the cases of different λ. In one case $\lambda = 0$ and the other $\lambda = 0.5$. It is noticed from Fig.4.1 that in both cases condition number grows algebraically with N.

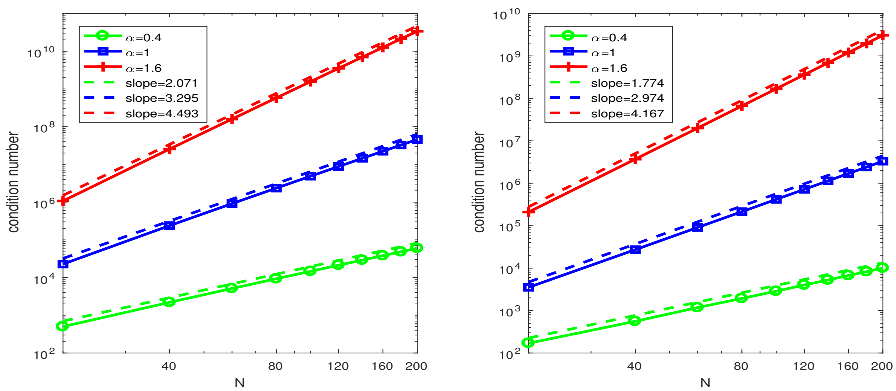

Figure 4.1: Condition number of the differentiation matrix for modified rational function versus N. Left: $\lambda = 0$. Right: $\lambda = 0.5$.

As with Hermite functions, we can also study the use of scaling and application to multi-term differential equations. We omit it here.

4.4 Differentiation matrix of the spectral collocation method with Lagrange bases

In the above section, we have derived explicit formulas for the differential matrices of using the rational-type bases by pseudo-spectral method. In this section, we shall discuss the spectral collocation method with Lagrange type bases. By using the Lagrange type bases, we approximate the solution in the following way

$$u_N(x) = \sum_{j=0}^{N-1} u_j l_j(x), \quad \text{with} \quad l_j(x_k) = \delta_{jk}, \quad 0 \leq j, k \leq N-1.$$

Here the Lagrange type bases $\{l_j(x)\}_{j=1}^{N}$ are defined as

$$l_j(x) = \frac{(1+x_j^2)^\beta}{(1+x^2)^\beta} \prod_{i=0, i \neq j}^{N-1} \frac{x - x_j}{x_i - x_j}, \quad 0 \leq j \leq N-1.$$

Here $x_i, i = 0, 1, ..., N-1$ are the transformed Gauss-Jacobi points. It is clear that we can express every Lagrange-type basis with rational functions $R_k^\lambda(x)$, i.e.,

$$l_j(x) = \sum_{k=0}^{N-1} b_k^j R_k^\lambda(x), \quad \text{with} \quad b_k^j = b_k^j = \frac{R_k^\lambda(x_j)\omega_j}{\gamma_k^\lambda}, \quad 0 \le j, k \le N-1.$$

where ω_j, $j = 0, 1, ..., N-1$ are the weights of the Gauss-Jacobi quadrature associated with Gegenbauer polynomials, i.e., $\alpha = \beta = \lambda - \frac{1}{2}$. Consequently, we can easily derive the associated differential matrix $\mathcal{D}^{L,\alpha,\lambda}$ with Lagrange type bases

$$\mathcal{D}_{i,j}^{L,\alpha,\lambda} = (-\Delta)^{\alpha/2} l_j(x_i) = \sum_{k=0}^{N-1} b_k^j (-\Delta)^{\alpha/2} R_j^\lambda(x_i). \tag{4.8}$$

The quantities $(-\Delta)^{\alpha/2} R_j^\lambda(x_i)$ can be obtained via (4.3) and (4.4).

In Fig.4.2, we present the condition number of this differential matrix with respect to the number of collocation points N, and test the cases of $\lambda = 0$ and $\lambda = 0.5$ as in former section. It is noticed from Fig.4.2 that in both cases condition number grows algebraically with N– $N^{2\alpha}$, which is in accordance of integer order differential equation, where the condition number for first and second order rational collocation methods are asymptotically N^2 and N^4, as demonstrated in [89].

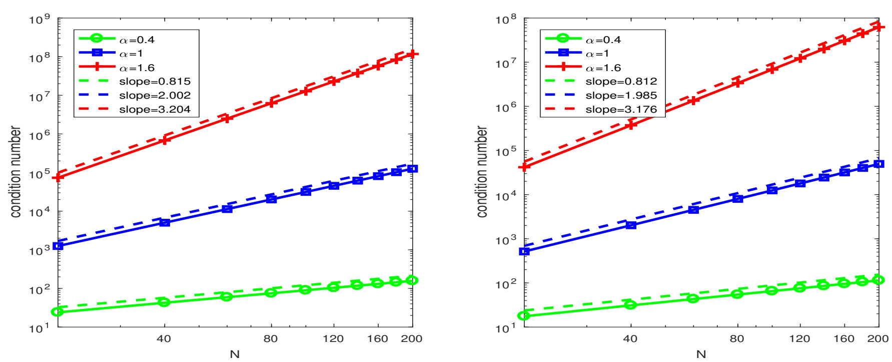

Figure 4.2: Condition number of the differentiation matrix for nodal expansion with modified rational function versus N. Left: $\lambda = 0$. Right: $\lambda = 0.5$.

4.5 Convergence analysis

Let u and u_N be the solution of (1.3) and its collocation method with the differentiation matrix of the fractional Laplace operator given by $\mathcal{D}_{i,j}^{L,\alpha,\lambda}$ in (4.8), then for modified Legendre rational function we have the following theorem.

Theorem 4.5 *Assume that $u \in H_C^{r_1}(\mathbb{R})$ and $f \in H_C^{r_2}(\mathbb{R})$ with $r_1, r_2 > 0$, there exists an integer $N_0 > 0$, s.t. for $N > N_0$, we have*

$$\left\|u - u_N\right\| \le \left\|u - u_N\right\|_{H^{\frac{\alpha}{2}}} \lesssim N^{\frac{\alpha}{2}+1-r_1}\left\|u\right\|_{r_1,C} + N^{1-r_2}\left\|f\right\|_{r_2,C}.$$

Proof. Recall that we collocate the equation on $N+1$ mapped Jacobi-Gauss points $\{x_j\}_{j=0}^N$ associated with the weight function $\omega(x) = 1$.

$$(-\Delta)^{\alpha/2} u_N(x_j) + \rho u_N(x_j) = f(x_j), \quad j = 0, ..., N.$$

Multiply both sides with $v_N(x_j)\omega_j$, where $v_N \in V_N^{\frac{1}{2}}(\mathbb{R})$, and sum up using the exactness of Gauss quadrature, we rewrite the scheme in the following variational form:

$$\left((-\Delta)^{\alpha/2} u_N, v_N\right)_N + c(u_N, v_N) = \left(I_N^{\frac{1}{2}} f, v_N\right). \tag{4.9}$$

where

$$(u_N, v_N)_N = \sum_{j=0}^{N} (-\Delta)^{\alpha/2} u_N(x_j)\, v_N(x_j)\, \omega_j.$$

Note that

$$\left((-\Delta)^{\alpha/2} v_N, v_N\right)_N \approx \left((-\Delta)^{\alpha/2} v_N, v_N\right)$$

and

$$\left((-\Delta)^{\alpha/2} v_N, v_N\right) = (|\xi|^\alpha \hat{v}_N, \hat{v}_N) \ge 0.$$

So there exists an integer $N_0 > 0$, such that for all $N > N_0$, we have

$$\left((-\Delta)^{\alpha/2} v_N, v_N\right)_N \ge 0, \forall v_N \in V_N^{\frac{1}{2}}(\mathbb{R}).$$

Define the bilinear form

$$a_\alpha(u, v) = \left((-\Delta)^{\alpha/2} u, v\right) + \rho(u, v).$$

Then for $N \ge N_0$, we have $a_\alpha(u, u) \ge 0$. Define the norm

$$\|u\|_\alpha := \sqrt{a_\alpha(u, u)}.$$

By definition, we have

$$\|u\|^2 \le a_\alpha(u, u) \lesssim \|u\|^2_{H^{\frac{\alpha}{2}}}, \quad a_\alpha(u, v) \le \|u\|_\alpha \|v\|_\alpha.$$

Compare (4.9) with the variational form of (1.3)

$$\left((-\Delta)^{\alpha/2}u, v_N\right) + \rho\,(u, v_N) = (f, v_N)\,, \tag{4.10}$$

and apply the Strang's first lemma 2.8, we obtain immediately

$$\left\|u-u_N\right\|_\alpha \lesssim \inf_{v_N\in V_N^{\frac{1}{2}}}\left\|u-v_N\right\|_\alpha + \left\|(-\Delta)^{\alpha/2}u - I_N^{\frac{1}{2}}\left((-\Delta)^{\alpha/2}u\right)\right\| + \left\|f - I_N^{\frac{1}{2}}(f)\right\|$$

Since

$$\inf_{v_N\in V_N^{\frac{1}{2}}}\left\|u-v_N\right\|_\alpha \le \left\|u - I_N^{\frac{1}{2}}(u)\right\|_\alpha \lesssim \left\|u - I_N^{\frac{1}{2}}u\right\|_{H^{\frac{\alpha}{2}}}.$$

and

$$\begin{aligned}(-\Delta)^{\alpha/2}u - I_N^{\frac{1}{2}}\left((-\Delta)^{\alpha/2}u\right) &= \left((-\Delta)^{\alpha/2}u + \rho u\right) - I_N^{\frac{1}{2}}\left((-\Delta)^{\alpha/2}u + \rho u\right)\\ &+ \rho\left(I_N^{\frac{1}{2}}(u) - u\right) = f - I_N^{\frac{1}{2}}f + \rho\left(I_N^{\frac{1}{2}}u - u\right).\end{aligned}$$

Using lemma 2.6, we have the desired result.

We can have similar result for modified Chebyshev rational function by using lemma 2.7 that

Theorem 4.6 *Assume that $u \in H_{A_1}^{r_1}(\mathbb{R})$ and $f \in H_{A_1}^{r_2}(\mathbb{R})$ with $r_1, r_2 > 0$, there exists an integer $N_0 > 0$, s.t. for $N > N_0$, we have*

$$\left\|u-u_N\right\| \le \left\|u-u_N\right\|_{H^{\frac{\alpha}{2}}} \lesssim N^{\frac{\alpha}{2}+1-r_1}\left\|u\right\|_{r_1,A_1} + N^{1-r_2}\left\|f\right\|_{r_2,A_1}.$$

4.6 Numerical examples

In this section, we shall present several examples to show the convergence property of our spectral collocation methods with modified rational functions. In all our computations, we shall report the numerical error both in the weighted norm e_w and in the maximum norm e_m, which are defined respectively as

$$e_w = \|u(x) - u_N(x)\|, \quad e_m = \max_j |u(x_j) - u_N(x_j)|\,.$$

Also for ease of computing Gauss points and corresponding weight, we only test the case with $\lambda = 0$ and 0.5, which correspond to the modified Chebyshev rational function and modified Legendre function respectively.

4.6.1 With exponential decay right hand side

Our first example is the fractional Laplace equation

$$\begin{cases} (-\Delta)^{\alpha/2} u(x) + \rho u(x) = f(x), & x \in \mathbb{R}, \\ u(x) = 0, & |x| \to \infty. \end{cases} \tag{4.11}$$

$\rho = 1$. We take the right hand side as $f(x) = \exp(-\frac{x^2}{2})(1+x)$. Since no exact solution is available, we use the numerical solution with $N = 200$ as the reference solution. Here we test the cases for $\alpha = 0.4, 1, 1.6$. Before presenting the results with modified rational function, we first give the numerical errors for generalized Hermite function, as described in last chapter, in Fig.4.3 in log-log scale.

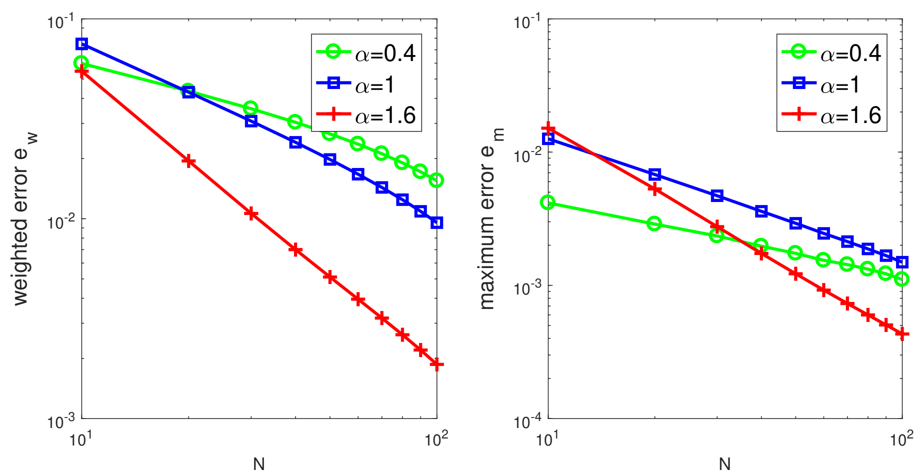

Figure 4.3: Numerical error for $f(x) = \exp(-\frac{x^2}{2})(1+x)$ with generalized Hermite function. Left: weighted norm. Right: maximum norm.

From Fig.4.3, algebraic convergence for weighted error and maximum error is observed. Then numerical errors with modified rational function for $\lambda = 0$ and 0.5 in log-log scale are given in Fig.4.4 and Fig.4.5.

From Fig.4.4 and Fig.4.5, algebraic convergence for weight error was observed. And compare to Fig.4.3, numerical errors with modified rational functional decay faster. Meanwhile the convergence rate improves as α increases.

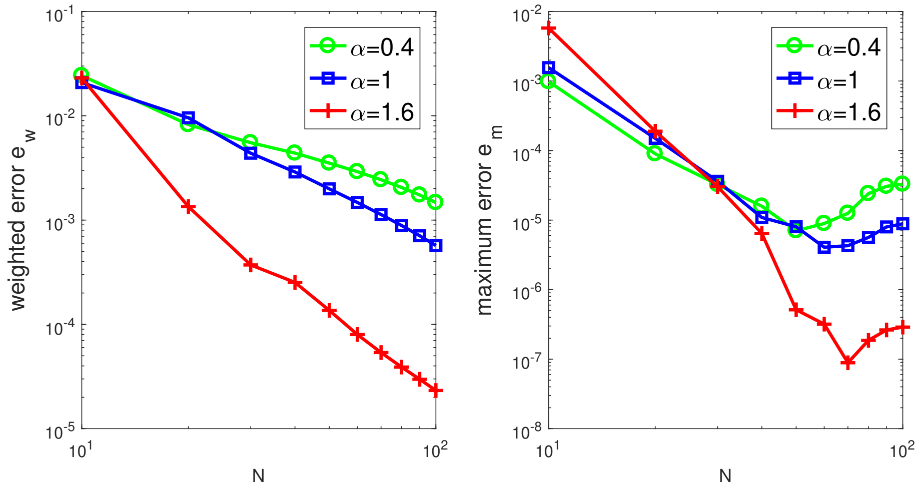

Figure 4.4: Numerical error for $f(x) = \exp(-\frac{x^2}{2})(1+x)$ with $\lambda = 0$. Left: weighted norm. Right: maximum norm.

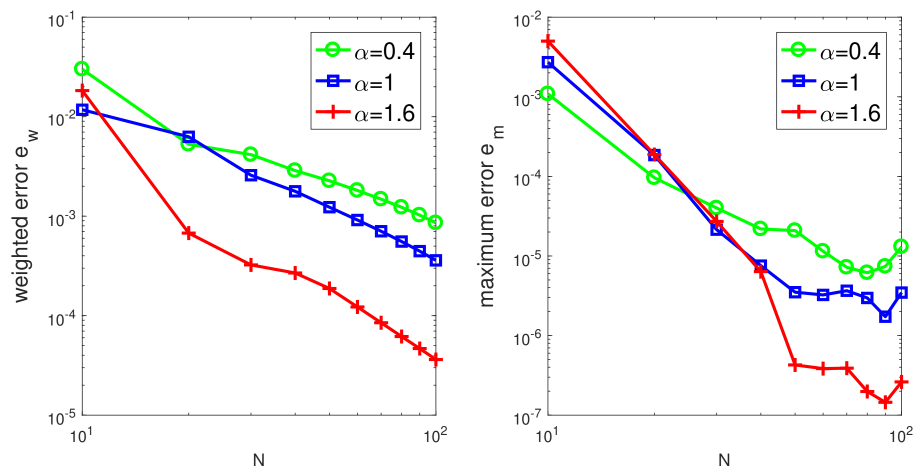

Figure 4.5: Numerical error for $f(x) = \exp(-\frac{x^2}{2})(1+x)$ with $\lambda = 0.5$. Left: weighted norm. Right: maximum norm.

4.6.2 With algebraic decay right hand side

Next, we consider the following linear fractional PDE

$$\begin{cases} (-\Delta)^{\alpha/2} u\left(x\right) + \rho u\left(x\right) = f\left(x\right), & x \in \mathbb{R} \\ u\left(x\right) = 0, & x \to \infty \end{cases} \tag{4.12}$$

$\rho = 2$. We take the right hand side as $f\left(x\right) = \frac{1}{(1+x^2)^2}$. As in former case, we first present the results generalized Hermite function in Fig.4.6.

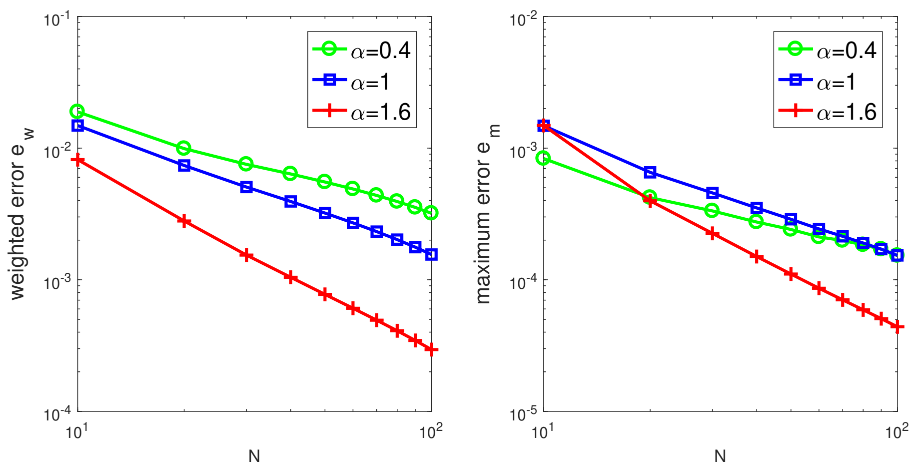

Figure 4.6: Numerical error for $f\left(x\right) = \frac{1}{(1+x^2)^2}$ with generalized Hermite function. Left: weighted norm. Right: maximum norm.

Then numerical errors are given in Fig.4.7 and Fig.4.8 Similar convergence behavior are obtained as the last example.

4.6.3 A multi-term fractional model

Our next example is the multi-term fractional Laplacian equation:

$$\sum_{j=1}^{J} \omega_j (-\Delta)^{\alpha_j/2} u(x) = f(x), \quad x \in \mathbb{R}. \tag{4.13}$$

Here we set $J = 4$ with $\{\alpha_j\}_{j=1}^{J}$ are chosen as the transformed Chebyshev-Gauss-Lobatto points

$$\alpha_1 = 0, \quad \alpha_2 = 0.5 \quad \alpha_3 = 1.5, \quad \alpha_4 = 2. \tag{4.14}$$

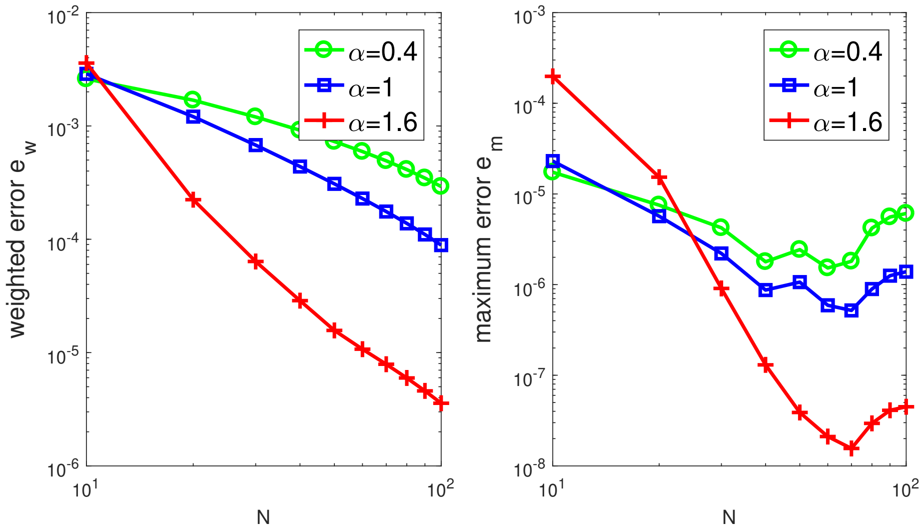

Figure 4.7: Numerical error for $f(x) = \frac{1}{(1+x^2)^2}$ with $\lambda = 0$. Left: weighted norm. Right: maximum norm.

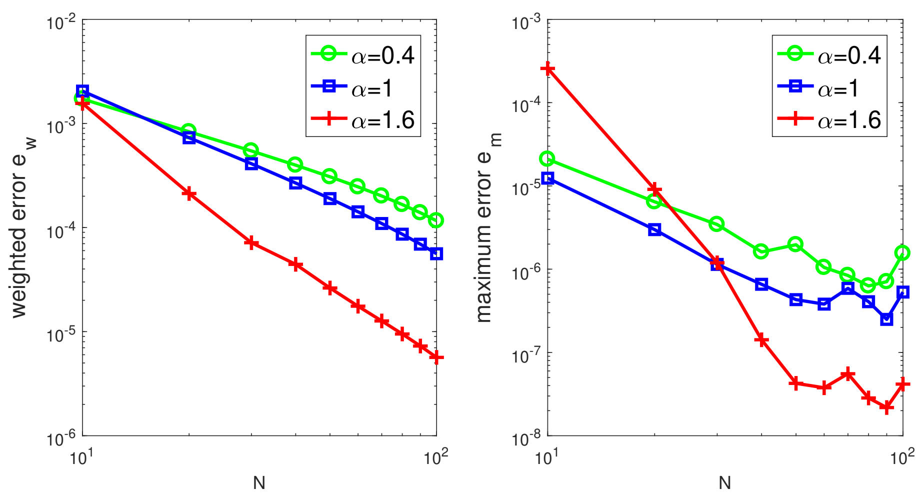

Figure 4.8: Numerical error for $f(x) = \frac{1}{(1+x^2)^2}$ with $\lambda = 0.5$. Left: weighted norm. Right: maximum norm.

and $\{\omega_j\}_{j=1}^{J}$ are the corresponding weight, i.e.,

$$\omega_1 = \frac{\pi}{6}, \quad \omega_2 = \frac{\pi}{3}, \quad \omega_3 = \frac{\pi}{3}, \quad \omega_4 = \frac{\pi}{6}. \tag{4.15}$$

We take the right hand side as $f(x) = \dfrac{x}{(1+x^2)^4}$. And we consider $\beta = 0.2$. Numerical errors are given in Fig.4.9 and Fig.4.10. Same convergence result is observed.

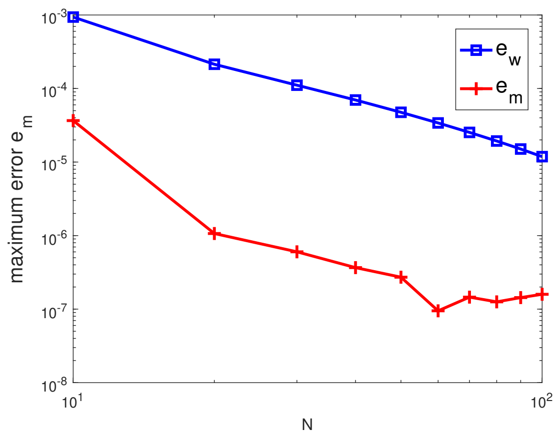

Figure 4.9: Numerical error for multi-term problem with $f(x) = \dfrac{x}{(1+x^2)^4}$ and $\lambda = 0$.

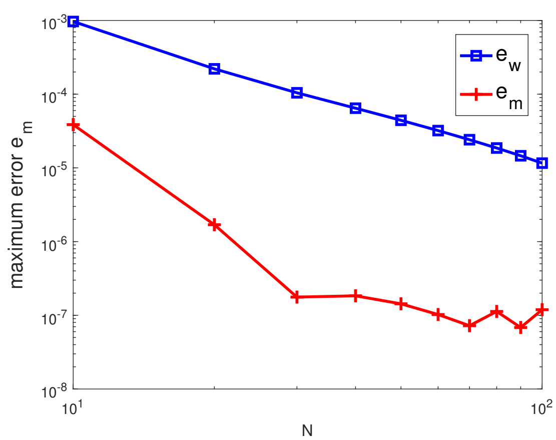

Figure 4.10: Numerical error for multi-term problem with $f(x) = \dfrac{x}{(1+x^2)^4}$ and $\lambda = 0.5$.

4.6.4 A nonlinear example

Our next example is a nonlinear fractional PDE

$$(-\Delta)^{\alpha/2}u(x) + r(x)u(x) = f(x) \tag{4.16}$$

Here we choose $r(x) = 1 + \exp(-x^2)$ and the right hand side $f(x) = \dfrac{\sin(x)}{(1+x^2)^3}$. We test the case for $\alpha = 0.4, 1, 1.6$. Numerical errors with modified Chebyshev rational functions and modified Legendre functions are given in Fig.4.11 and Fig.4.12. As in former cases, similar results are observed here.

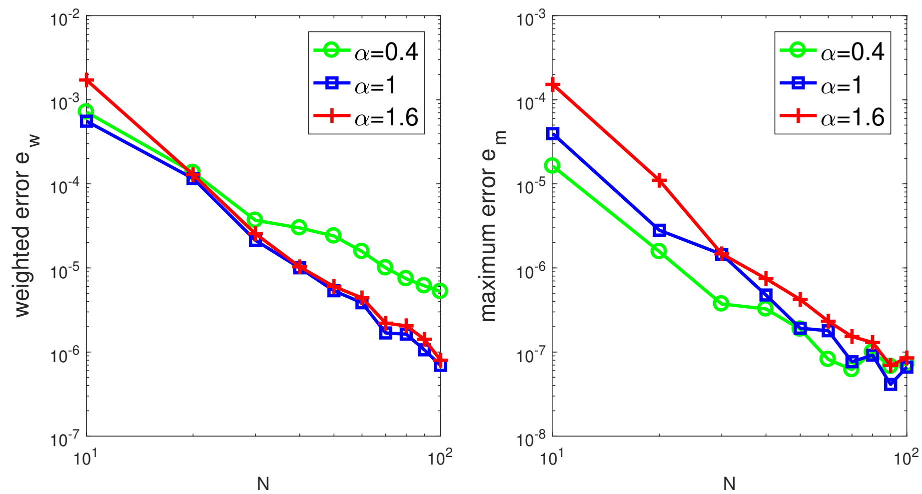

Figure 4.11: Numerical error for nonlinear equation with $f(x) = \dfrac{\sin(x)}{(1+x^2)^3}$ and $\lambda = 0$. Left: weighted norm. Right: maximum norm.

4.6.5 An eigenvalue problem

Finally we consider again the following eigenvalue problem

$$\left((-\Delta)^{\alpha/2} + x^2\right)u(x) = \lambda u(x) \tag{4.17}$$

where the eigenvalues with with $\alpha = 1$ are explicitly given in [42] as in last section. In this example, we shall compute the first three eigenvalues by the spectral collocation method. The exact eigenvalues are

$$\gamma_1 \approx 1.01879297164747, \quad \gamma_2 \approx 2.33810741045976,$$

$$\gamma_3 \approx 3.24819758217983.$$

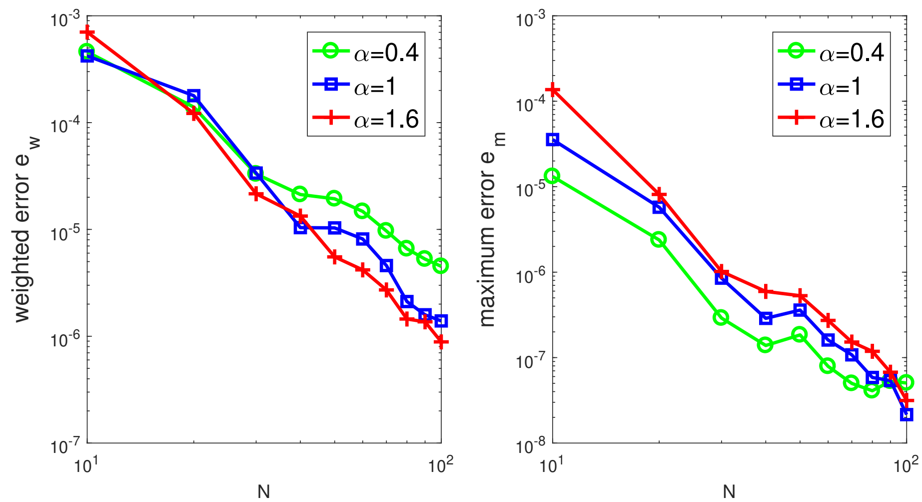

Figure 4.12: Numerical error for nonlinear equation with $f(x) = \dfrac{\sin(x)}{(1+x^2)^3}$ and $\lambda = 0.5$. Left: weighted norm. Right: maximum norm.

We take $\lambda = 0$, and 0.5. Numerical error of the first three eigenvalues are given in Fig.4.13 and Fig.4.14.

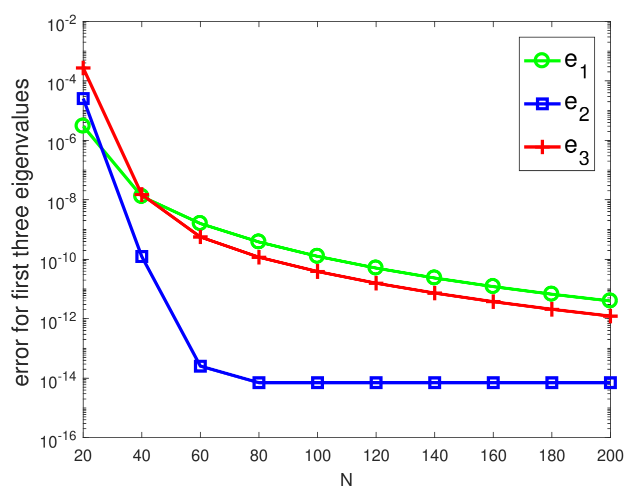

Figure 4.13: Numerical errors for the first four eigenvalue with $\lambda = 0$.

Comparing with Fig.3.14 in last chapter with generalized Hermite function, here smaller errors are got for the eigenvalues with modified rational functions. This improvement may be explained by the non-exponential property of eigenfunctions.

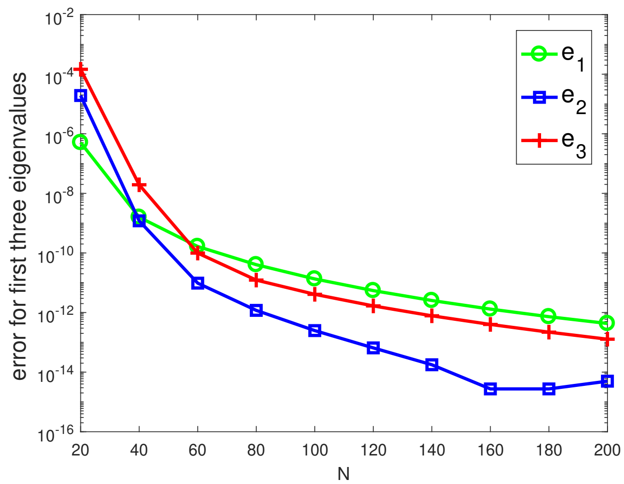

Figure 4.14: Numerical errors of the first four eigenvalue with $\lambda = 0.5$.

4.7 Concluding remarks

In this chapter, we proposed the spectral collocation method with modified rational functions that is well suited for solutions that decay algebraically in infinity. Convergence analysis for special cases are derived, i.e., the modified Chebyshev rational function and the modified Legendre rational function. We also provide numerical examples to demonstrate the efficiency. Meanwhile, application to multi-term problems and use of scaling parameter are straightforward.

Here are two main problems to be considered:

- Application to higher dimensions with modified rational functions. As we already have proposed Hermite functions for two dimension, the next step is for modified rational functions.

- Convergence analysis for modified rational functions with arbitrary parameters. Only the error estimates for the modified Chebyshev/Legendre rational functions are derived, we shall then do the same for general modified rational functions.

Chapter 5

Summary and future work

Fractional differential equations are naturally derived on unbounded domains. In this thesis, we have proposed spectral collocation methods for fractional differential equations in unbounded domain for two basis, i.e., the Hermite type basis and the rational function type basis, corresponding to different decay rate of solutions. Convergence analysis and numerical examples are also provided.

Based on Hermite polynomials, we first construct spectral collocation methods for over-scaled Hermite function $\widetilde{H}_n(x)$ and generalized Hermite function $\widehat{H}_n(x)$. The fractional Laplacian of over-scaled Hermite function is represented by confluent hypergeometric function, while for generalized Hermite function, the result is a finite sum of confluent hypergeometric functions. We also provide tensorized 1D bases for two dimension. The first basis with over-scaled Hermite function provides some insight on how to deal with the other. It is observed that the generalized Hermite function behaves better than the over-scaled Hermite function both in terms of condition number and ease in convergence analysis.

The second basis is the modified rational function. We start from Jacobi polynomials $J_n^{\alpha,\beta}(t)$ on bounded domain $[-1,1]$, and then we use an algebraic mapping

$$t = \frac{x}{\sqrt{1+x^2}}, \quad x = \frac{t}{\sqrt{1-t^2}}$$

which gives mapped Jacobi polynomials $j_n^{\alpha,\beta}(x)$. For convenience, we start from Gegenbauer polynomials $C_n^{\lambda}(t)$, which are special cases of Jacobi polynomials with the two parameters being equal, i.e., $\alpha = \beta = \lambda - \frac{1}{2}$, and also generalize Chebyshev and

Legendre polynomials. After transformed to unbounded domain, the term $\frac{1}{(1+x^2)^{\frac{\lambda+1}{2}}}$ will be multiplied so that the weight function of the modified rational functions becomes 1. This can also make convergence analysis simplier. It is interesting to demonstrate that the fractional Laplacian of the modified rational functions are a finite sum of hypergeometric function.

Although confluent hypergeometric and hypergeometric functions are defined by power series or integral, which may not be very easy to compute, we have shown in both cases that recurrence relations can be used to compute the differentiation matrix. This makes the computation of the differentiation matrix much easier. Use of scaling parameter and application to multi-term and nonlinear differential equations are also included.

There are still some issues to be investigated:

- Higher dimensions for modified rational functions. One possible way may be to transform the ordinary differential equation from Cartesian coordinates to polar coordinates as described in [74] for multi-dimensional domains.

- Convergence analysis for modified rational functions with arbitrary parameters. For the convergence analysis in Chapter 4, we only derive the error estimates for the modified Chebyshev/Legendre rational functions. In order to derive similar results for modified rational functions, we may need to define new Sobolev spaces and norms as was done in [34, 88].

- Time dependent problems. In this thesis, only steady problems are concerned. The next step is to consider time-dependent problems such as fractional advection-dispersion equation, fractional Schrodinger equation, and fractional phase filed problems.

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July 2018